AFAL TR-87-063

AD:

(12)

Final Report
for the period
1 October 1984 to
30 June 1987

Prediction of Molecular Properties
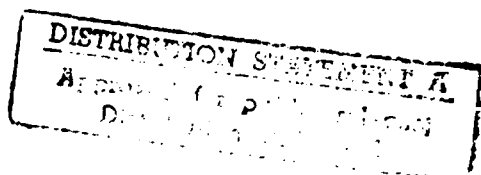
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FOREWORD

This final report on the in-house project Prediction of Molecular Properties was prepared by the Air Force Astronautics Laboratory (AFAL), Edwards Air Force Base, CA. The period of the report is 1 October 1984 to 30 June 1987. AFAL Project Manager was Lt Walt Lauderdale.

This technical report has been reviewed and is approved for distribution in accordance with the the distribution statement on the cover and on the DD Form 1473.

WALTER J. LAUDERDALE, 1Lt, USAF
Project Manager

FOR THE COMMANDER

ROBERT C. CORLEY
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REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED		1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for Public Release. Distribution is unlimited.
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE		
4. PERFORMING ORGANIZATION REPORT NUMBER(S) AFAL-TR-87-063		5. MONITORING ORGANIZATION REPORT NUMBER(S)

6a. NAME OF PERFORMING ORGANIZATION Air Force Astronautics Laboratory	6b. OFFICE SYMBOL (If applicable) CX	7a. NAME OF MONITORING ORGANIZATION
6c. ADDRESS (City, State and ZIP Code) Edwards AFB CA 93523-5000		7b. ADDRESS (City, State and ZIP Code)

8a. NAME OF FUNDING/SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
8c. ADDRESS (City, State and ZIP Code)		10. SOURCE OF FUNDING NOS.

11. TITLE (Include Security Classification) PREDICTION OF MOLECULAR PROPERTIES (U)	PROGRAM ELEMENT NO 62302F	PROJECT NO. 5730	TASK NO. 00	WORK UNIT NO. RH

12. PERSONAL AUTHOR(S)
Lauderdale, Walter J., and Rodgers, Stephen L.

13a. TYPE OF REPORT Final	13b. TIME COVERED FROM 84/10/1 TO 87/6/30	14. DATE OF REPORT (Yr., Mo., Day) 87/8	15. PAGE COUNT

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB. GR.	Molecular Mechanics, MM2, Semi-Empirical, MOPAC, MINDO/3,
07	04		MNDO, AMI, an initio, Gaussian 82, GAMESS, Nitro, Nitramine,
09	02		Computational Chemistry, 2,6-Diamino-3,5-dinitropyrazine.

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

This project was conducted to establish a computational capability at the Air Force Astronautics Laboratory and to evaluate its applicability to chemical problems of interest to rocket propulsion. The three types of methodologies implemented were molecular mechanics, semi-empirical, and ab initio. The specific programs installed were MM2 (molecular mechanics, MOPAC (semi-empirical), GAMESS (ab initio), and Guassian 82 (ab initio). New parameters for nitro and nitramine moieties were developed for MM2. The performance of the MOPAC methods (MINDO/3, MNDO, and AMI) on nitramine-containing compounds was evaluated and found to provide good molecular geometries, but inconsistent of heats of formation. GAMESS and Gaussian 82 were installed and evaluated on their applicibility to various molecular systems of propulsion interest.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☒ DTIC USERS ☐	UNCLASSIFIED

22a. NAME OF RESPONSIBLE INDIVIDUAL Walter J. Lauderdale, 1Lt, USAF	22b. TELEPHONE NUMBER (Include Area Code) (805) 275-5413	22c. OFFICE SYMBOL CX

18. 7-Amino-4,5,6-trinitrobenzofuroxan; Benzotrifuroxane; 1,4-Dinitro- [3,4-b] ,[3,4-e]

difurazanopiperazine; Dinitrofurazane; 4-Methyl-1,3-dinitro-1,3-diazacyclopentane;

Pentanitroaniline; 6,6,8-Trinitropentacyclo $[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]$ decane; Bis(2-fluoro-2,

2-dinitroethyl)nitramine; 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane; 1,1,1,3,6,8,8,

8-Octanitro-3,6-diazaoctane; 1,3,5-Trinitro-1,3,5-triazacyclohexane; 1-Nitroso-2,2-di

(trifluoromethyl)-1,3-diazacyclopentan-4-one; 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-

2,4,6,8-tetraazabicyclo [3.3.0] octane; 1,3,5-Tribenzamido-1,3,5-hexahydrotriazine;

1-Benzoyl-4-benzamido-.delta.^{2}-1,2,4-triazoline; Bis-tetrazolo[1,5-a:1',5'-c]pyrazine;

1,4-Dinitro-2,3,5,6-tetrabromo-2,3,5,6-piperazine; 7-Nitro-5,6-dihydro-7H-imidazolo

[1,2-d] tetrazole; 6,6,10,10-Tetranitropentacyclo $[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]$ decane; 1,3,5,5-

Tetranitrohexahydropyrimidine; Nitramide; Dimethylnitramide

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INTRODUCTION

Prediction of Molecular Properties wa, conducted to bring a computational chemistry capability to the Air Force Astronautics Laboratory (AFAL). Computational chemistry is the application of theoretical chemistry (quantum mechanics, force field theory) to achieve an understanding of molecular behavior. It can be used to explore properties of molecular systems that would otherwise be hard or impossible to determine experimentally. In addition, one can conjecture new, unknown molecules and determine their properties (and hence their usefulness) without going through an expensive synthesis effort. Such a capability can be exploited to increase the efficient use of a chemist's time. Methods for computational chemistry have grown in both accuracy and complexity over the last 10 years through advances in algorithms and computers.

This computational capacity provides for the determination of a variety of molecular properties. These include, but are not limited to, geometries, total energies, electron distributions, heats of formation, and vibrational analyses. Of particular interest to the AFAL are reaction kinetics, transition states, infrared (IR) signature, decomposition products, and chemical reactivity. Several different approaches are available to obtain these answers includeing molecular mechanics, semi-empirical molecular orbital, and ab initio methods. Each of these has its own strengths and weaknesses, but together they provide a powerful set of tools for the practicing chemist.

This project installed several computer programs on AFAL's facilities. They are the molecular mechanics program Molecular

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Mechanics 2 (MM2) [Ref. 1], the semi-empirical program MOPAC [Ref. 2], the ab initio program Gaussian 80 [Ref. 3], its follow-on, Gaussian 82 [Ref. 4], and the ab initio program GAMESS (General Atomic and Molecular Electronic Structure System) [Ref. 5]. MM2 required additional parameters to perform calculations on molecules of interest and these were developed. MOPAC was evaluated on its performance for molecules of interest with no additional parameterization attempted. However, a database of completed computations on molecules containing nitro and nitramine groups was compiled for use by other groups involved with parameterization. The Gaussian and GAMESS programs were evaluated on their self-contained basis sets for accuracy and applicability. All these programs can answer some very important chemical questions. In particular, they can help determine reaction mechanisms and the stabilities of a variety of compounds.

BACKGROUND

The programs selected for use in this project had to meet several criteria. The most important consideration of all was the applicability of the programs to compounds of interest to the AFAL. These include polymers, energetic polymers, nitrated and nitramine compounds, and high energy density matter (HEDM). In addition, three other criteria were: how widespread and accepted is the program in the chemical community, ease of use, and degree of difficulty in implementing improvements. The criteria are listed in priority order. Programs selected are ones which are utilized and improved by other groups and will be described in detail.

MOLECULAR MECHANICS (MM2)

There are many situations in which an experimental chemist would like to know more of the detailed nature of molecular structure, especially conformation. A more accurate interpretation of [1]H-nuclear magnetic resonance (NMR) coupling constants or circular dichroism curves, for example, is particularly facilitated by a knowledge of low energy molecular geometry. There are several ways this knowledge can be obtained, e.g., through such experimental methods as X-ray crystallo-graphy, electron diffraction, microwave, and vibrational spectroscopy. Unfortunately, many of these methods are difficult or require special equipment and training. The X-ray crystallography method also yields a crystal structure which may be significantly different from the gas phase or solution structure, where most reactions occur.

An alternative approach to experimental determinations of molecular structures employs selected computational methods. Of the three methods of calculation, the ab initio method is the most basic, starting from first principles of quantum mechanics. While ab initio calculations are usually quite reliable, the computer time necessary for a full geometry optimization is so large that molecules possessing more than 10 non-hydrogen atoms are practically impossible to calculate. Semi-empirical MO methods are capable of performing calculations on larger molecules, at a faster rate than ab initio calculations. However, semi-empirical MO calculations are still too slow to handle many of the molecules of experimental interest. They also suffer the limitations of approxi-mations introduced to improve the computational speed [Ref. 6]. A third computational method is the force field calculation, also known as the

Westheimer or molecular mechanics method. This is a purely empirical method, based not on theoretical considerations, but on experimental results. This pragmatic approach produces a calculation method which is faster and often as accurate, if not more accurate, than the other approaches. It places a tool in the hands of the experimental chemist which is both easy to use and reliable. Several good reviews of the force field method have been published [Refs. 6-9].

Philosophy of Force Field Calculations

Quantum mechanical methods, such as ab initio calculations, all involve calculations of the electronic system after the nuclear positions have been fixed, or assumed. To obtain accurate results the electronic calculations must be repeated with different nuclear positions until an energy minimum is found. The force field method takes the opposite approach. It is concerned with the positioning of the nuclei, while the electronic effects are only indirectly taken into consideration. Oftentimes the two approaches are combined using the force field method to obtain the starting nuclei positions for the quantum mechanical calculations.

The molecule is considered a collection of atoms held together by an elastic force, much like a ball on a spring. This elastic force can be described by potential energy functions of the structural features; such as bond lengths, bond angles, nonbonded interactions, and other such features. The sum of these potential energy functions forms the force field.

The molecular force field energy arises from the difference of idealized structural features and those features made to fit the

structural constraints of the molecule as calculated. This energy, "E",
sometimes called the "strain energy" of the molecule, arises from the
sum of the stretching or compression energy, "E_s", where the molecular
bonds are being changed from their natural bond length; the bending
energy, "E_b", where the bonds are being bent from their natural values;
the torsional energy "E_ω", due to twisting of the bonds; and the
nonbonded interaction energy, "E_{nb}". Other energy potentials may be
added, such as electrostatic repulsions or hydrogen bonding. In
general, there is no standard as to what potential energy functions to
include; consequently, there are many different molecular mechanics
force fields now in use.

It is important to note that the strain energy, "E", is only a
comparison to a hypothetical ideal situation. In itself, "E" has no
physical meaning. Each component of "E" will change depending on which
parameters are used and their functional form. The individual values
are interrelated and must not be used independently. What is important
is the sum of all the contributions.

Each potential energy function is constructed in such a way as to
duplicate experimental results. Parameters are formulated for each
structural feature of the molecule and for each type of atom which may
be part of the molecule. It is this parameterization which leans
heavily on experimental data. It is also this parameterization which
determines the degree of accuracy of the calculated results. Obviously,
those molecules which most closely resemble that data set will be
calculated most accurately.

Considerable experimental data are available for the structure of
small molecules. Empirical equations can be formulated using these data

to describe these structural features. A large molecule consists of the same elements as small molecules put together in various ways. It is assumed that those properties of the small molecules may be combined to form larger molecules. This combining is what force field calculations attempt to do.

The main strength of the force field method is its speed and ease of application. Its main drawback is the need for a large database, similar to the molecule to be calculated. Once available, however, this dependence on large databases is an assurance of reliability.

The Mechanical Model

The most widely used force field method is the program developed by N.L. Allinger. There are three versions of this program: MM1, MM2, and MMP1 [Ref. 6]. MM1 and MMP1 are parameterized for saturated hydro- carbons, nonconjugated olefins, alkynes, and various heteroatoms. MMP1 is a version of MM1 with an algorithm for calculating conjugated pi systems. MM2 [Ref. 1] is an updated (1980) version of MM1, with improved parameters. The MM2 version treats hydrogens as smaller and softer and carbons larger than the older program. In addition, it also includes a 2-fold torsion term for the butane type carbon system. The VAX version of MM2 was used to perform all calculations reported here. The following discussion of the force field model will refer specifi- cally to the MM2 program, though it also applies in general to most force field methods.

Force field calculations are done on "molecular models" [Ref. 8]. These models are assigned properties which reproduce experimental facts. It is important to note that these models do not truly represent the

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molecule in its entirety, but only in that the particular experimental

data set which was used to construct the model is reproduced. Thus,

models built on one type of database usually are very accurate in

producing reliable results for those particular properties, and less

accurate in producing properties from which they were not parameterized.

There are two general kinds of force fields now in use [Ref. 10];

the valence force field and the Urey-Bradley force field. Both of these

methods seem to yield results that are essentially equivalent [Ref. 11].

The difference in the two force fields is that the valence theory

neglects 1,3 interactions.

Any deviation from the "natural" bond lengths and angles results in

an increase of energy. The amount of energy involved can be calculated

by applying Hooke's Law. Each energy change due to deviation is summed

over each bond length or bond angle to give the corresponding E_s and E_b

contribution. There are several considerations and refinements that

should be noted about employing Hooke's Law.

It takes more energy to stretch a bond than to bend it by about a

factor of 10. Consequently, if a molecule is distorted, most of the

distortion is found in the bond angles rather than in the bond lengths.

This is taken into account in the equations by setting the force

constant for bending, k_b, comparatively smaller than that for

stretching, k_s.

There is a tendency for Hooke's Law to overestimate the energy

involved in large distortions. This is because in large distortions

there is less overlap of the sp^3 orbitals, effectively reducing the

force constants. This problem is solved by adding cubic terms to the

Hooke's Law equation [Ref. 7].

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$$E_s = \Sigma \tfrac{1}{2} k_s (1 - 1_o)^2 \qquad\qquad E_b = \Sigma \tfrac{1}{2} k_\theta (\theta - \theta_o)^2 \qquad (1)$$

E_s = stretching energy $\qquad\qquad E_b$ = bending energy

1 = bond lengths $\qquad\qquad\qquad \theta$ = bond angles

k_s = force constant $\qquad\qquad\quad k_\theta$ = force constant

It should also be recognized that when a bond angle is compressed the two associated bond lengths become longer. The MM2 program handles this fact by including a "cross term", E_{sb}, the stretch-bend energy.

A final point is that the in-plane and out-of-plane force constants can be distinguished at sp^2 hybridized carbons. These become especially important in molecules, like cyclobutanone, where the ring bond angles are less than 120 degrees. This refinement is taken care of in the individual type parameters.

The next potential energy contribution to be considered is that from the rotation about the bonds. This internal rotation is most often expressed in terms of "torsional angle", ω. The energy barrier of rotation is most commonly described by the Fourier series, and is an indication of how the energy of the molecule changes with the rotation about the torsion angle. The equation is listed below.

$$E_\omega = \Sigma [\tfrac{1}{2} V_1 (1 + \cos \omega) + \tfrac{1}{2} V_2 (1 - \cos 2\omega) + \tfrac{1}{2} V_3 (1 + \cos 3\omega) + \ldots] \qquad (2)$$

E_ω = torsional energy $\qquad \omega$ = torsion angle

V = force constants

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The sum is over all the sequence of bonded atoms, which is part of the data that must be supplied MM2. The series is usually truncated after the third term. The constants V_1, V_2, and V_3 are arbitrarily chosen to fit the experimental data set. V_2 is the term describing rotation about double bonds and, therefore, is quite high.

In general, it takes less energy to distort a dihedral angle than to bend or stretch bonds, so molecular conformational changes will show up to a greater extent in torsional distortion.

The fourth potential energy term is for nonbonded interactions. As two atoms approach each other, there is first an attraction, due to London dispersion forces, and then a repulsion, from van der Waals interactions, as the atoms get too close. In MM2, Allinger uses the Hill equation to describe these interactions:

$$E_{vdw} = \varepsilon[-c_1(r\star/r)^6 + c_2 \exp(-c_3/r\star)] \tag{3}$$

E_{vdw} = van der Waals energy ε = energy parameter

r = interatomic distance c = constants

The c's are universal constants and ε and $r\star$ are atom-dependent parameters. The value for ε is calculated from the square root of the product of the epsilon parameter describing the "hardness" of the particular atom and the parameter describing the depth of the potential energy well. The hardness of an atom is related to the steepness of the repulsive segment of the potential well. The value $r\star$ is the sum of the van der Waals radii of interacting atoms. The sum is over all pairs of atoms not bonded to each other or to a common third atom. These curves

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are typically derived from nonbonded contact distances in crystalline hydrocarbons or using van der Waals data from real gases. Parameters for other atoms are then obtained by extrapolating or interpolating.

Considerations in Use of Molecular Mechanics Programs

Molecular mechanics programs can be designed to produce vibrational frequencies as well as molecular geometries. Allinger's MM2 program calculates only molecular geometries and associated strain energies. Thus MM2 would not be the method of choice for comparison to experimental spectral data. Other molecular mechanics programs are available to produce vibrational frequency data [Ref. 12].

MM2 produces the low energy geometry of a molecule by altering the three-dimensional coordinates of the molecule until a lower energy is obtained. The minimization scheme used is a modified Newton-Raphson energy minimization algorithm that moves individual atoms to reach optimized geometry [Ref. 7]. This process is repeated until the energy cannot be lowered further. There is one pitfall in this approach, however. In many molecules there is more than one energy well that the program can fall into, and this prevents further minimization to the absolute lowest well. Care must be taken to ensure that the calculated energy is indeed the lowest energy structure. To escape an energy well the coordinates must be altered to distort the geometry, and then further minimization can continue.

The input data for the program consists of, among other things, the beginning three-dimensional coordinates for the molecule. These can be obtained in several ways. For example, X-ray or microwave data can often be used. MM2 has available an option to convert crystal

coordinates to cartesian coordinates. There are also programs available from QCPE that will produce rough starting coordinates. For the calculations reported here the program CART [Ref. 13] which produces cartesian coordinates from geometrical relationships as measured on Dreiding models was used to obtain starting coordinates not available elsewhere. MM2 also has an option available where substituents may be added by the program to molecules being calculated. Many molecules can be formed from basic components of a molecule by using this option. For example, other molecules that contain a six-membered ring can be formed starting from cyclohexane.

MM2 has available a dihedral driver where a particular dihedral angle can be driven through a series of angles, or the angle can be fixed at other than the calculated low energy angle. This option is quite useful for determining rotational barriers or energy differences between conformers. It is also useful for escaping energy wells which are not the absolute lowest well.

The results of molecular mechanics calculations are only as good as the parameters used by the program. MM2 has been shown to have a highly reliable parameter set for several categories of molecules. The structural types that are of concern in this study are amines, nitro, and nitramine compounds. These chromophores are of particular interest because of their occurrence in energetic materials. There is no doubt, however, that the nitrogen containing groups such as the amines have been the most difficult to parameterize and use in the force field model. While accurate models for amines have recently been developed [Ref. 9], virtually no nitramine or nitro parameters are available. The difficulties with nitrogen arise from the lone pair in the sp^2 systems

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and the combination of the sp^3 and sp^2 nitrogens in the nitramine. A nice feature of MM2 allows the user to input missing parameters. With this feature, a set of parameters for a specific system could be developed. Parameters were therefore developed and used in the calculations.

There have been numerous cyclic ketone studies using MM2 that have produced very accurate results [Ref. 7]. MM2 calculations have been used to investigate the three-alkyl ketone effect [Ref. 14], conformations of medium-sized rings [Ref. 15], and conformational studies of cyclohexanone [Ref. 16], all with good results. It has also been shown that MM2 produces good results with ketones containing alpha methyl groups [Ref. 17]. MM2, then, seems to be a good tool with the proper parameterization for the calculation of the various other portions of the systems that are of interest in this study. Combined with the developed parameters, MM2 is capable of producing quick geometries and relative energies for systems of interest to the energetic material community.

Installation of MM2

The MM2 version received compiled readily on the VAX computer. However, in order to take advantage of the capabilities of the VAX command language (DCL), the OPEN statements were changed to not look for a specific file. The assignment of files to particular Fortran units was handled by the VAX operating system (see details about ASSIGN in the MOPAC installation section). No other modifications were necessary to operate the program.

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Force Field Parameterization

MM2 employs force field parameters that are derived from experimental observations, quantum mechanical computations and, sometimes, a combination of both. While the parameters are fairly empirical in their derivation, molecular mechanics calculations have been shown to achieve a high degree of chemical accuracy for those compounds for which parameters have been developed. MM2 differentiates elements and element groupings according to their environment. For example, a carbon in a simple alkane is defined differently than a carbon in a carbonyl group. Each atom type has its own set of force field parameters which are assumed to be applicable to any molecule containing a similar environment.

MM2 was obtained in order to perform computations on nitramine and nitro compounds. These are commonly used in propellant formulations, but are not so commonly used within the chemical community. As a result, virtually no MM2 results on nitramines and very little on nitro compounds have been reported in the literature. Therefore no parameters were available and had to be developed at the AFAL. The precision of the needed parameters depends on the end application. The nitramine and nitro computations were intended to be used primarily to obtain molecular geometry and relative energies. The parameters developed reflect that end use.

The required force field parameters missing from the MM2 program were those for the >NNO2 group. Atom types, bond length, bond angle, and torsional parameters all had to be developed. The amine nitrogen of the nitramine group was modeled by using the sp^2 nitrogen from amines (atom type 9 in MM2) and employing those specific

parameters. The oxygens were modeled by assuming them to be the same as a carbonyl oxygen (atom type 7) since both N-O bonds in the nitro group have substantial double bond character. The nitro nitrogen is sufficiently different from any other type of nitrogen that a new atom type was defined. The nitro nitrogen was defined as atom type 29 within the program. Additional atoms involved in the parameterization are sp^3 carbon (atom type 1), hydrogen (atom type 5), and fluorine (atom type 11).

As described earlier, there are several kinds of parameters required. The van der Waals parameter for atom type 29 was assumed to be the same as for the other nitrogen atom types (R = 1.820 Å, ϵ = 0.055 kcal/mole, atomic weight = 14.003 a.u.). The other parameters relating to bond lengths, bond angles, and torsional terms are obtained initially from experimental data or from well considered estimates. Specific parameterization procedures and algorithms for their development are well described in the literature and are relatively straightforward [Refs. 9,18,19]. The initial parameter values are included with the standard input file and variables are set which tell MM2 to read in the parameters. The process of parameterization is essentially an iterative one. The results of the calculation are compared to experiment for the model compounds and the parameters adjusted. The bond length parameters are adjusted first to achieve a good fit with experiment. Next, the bond angle parameters are changed. This is because the bond angles are affected by the repulsion between bonds defining the angles. Lastly, the torsional parameters are modified, since they depend on both bond lengths and bond angles.

Results

The parameterization process described above was followed to optimize the new parameters. Several model compounds were used to evaluate the results of the parameterization. These compounds were 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) [Ref. 20], 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) [Ref. 21], N,N-dimethylnitramide (DMN) [Ref. 22], and 1,1,3,5-tetranitrohexahydropyrimidine (DNNC) [Ref. 23]. Average values for selected bond lengths and bond angles are shown in Table 1.

TABLE 1. Average values for selected bond lengths (diatomic representation, in Angstroms) and bond angles (triatomic representation, in degrees) for some nitramines.

	RDX		HMX		DMN		DNNC	
	Cal'd	Exp[a]	Cal'd	Exp[b]	Cal'd	Exp[c]	Cal'd	Exp[d]
C-N	1.46	1.45	1.45	1.47	1.45	1.46	1.48	1.47
N-N	1.37	1.38	1.36	1.36	1.36	1.32	1.35	1.39
N-O	1.20	1.21	1.20	1.22	1.20	1.24	1.21	1.20
C-N-N	114.7	117.9	117.5	119.6	115.3	117.4	118.2	118.6
C-N-C	120.1	114.8	123.9	119.2	121.3	124.2	123.4	116.1
O-N-N	117.7	117.2	116.1	117.8	117.9	118.4	117.7	116.8
O-N-O	124.2	125.5	123.7	124.3	124.1	123.3	123.9	123.7

[a] See reference 20. [b] See reference 21. [c] See reference 22. [d] See reference 23.

The C-N bonds are reproduced very well, all to within 0.02 Å. The N-N bonds produced mixed results. The cyclic nitramines RDX and HMX showed excellent agreement, while the cyclic nitramine DNNC did not fare so well. This is most likely due to the presence of a geminal dinitro carbon which is beta to the two nitramine moieties in DNNC rather than another nitramine group as in RDX and HMX. This lack of additional nitramine groups is also present in DMN and probably accounts for its

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error as well. The N-O bonds are reproduced well except for DMN. The error is created by the lack of additional electron withdrawing groups beta to the nitramine moiety.

The bond angles are extremely well reproduced. The accuracy is to within 2.5° except for the C-N-N angles in RDX and all C-N-C angles. In the RDX case, the error is only a bit larger, being 3.2°. The C-N-C angles, however, presented a problem. Adjusting the parameters for this angle will affect the results obtained for the C-N-N angles. This tradeoff culminated in a balance between the two parameters. The results shown are the best that could be obtained when considering both types of angles. The C-N-N angles are more important to the particular moiety of interest ($>NNO_2$) than the C-N-C angles, so its accuracy received precedence.

The energy data is shown in Table 2. MM2 calculates what it calls "steric energy". This can roughly be equated to the heat of formation (ΔH_f) of a compound. While not very accurate, it appears to consistently overestimate the energy. Also, at least for RDX and HMX,

TABLE 2. Calculated steric energies and experimental heats of formation (ΔH_f) for selected nitramines in kcal/mole.

	Steric energy (cal'd)	ΔH_f(experimental)
RDX	26.3	14.7[a,b]
HMX	36.7	17.9[a,b]
DMN	6.5	-3.2[b,c]
DNNC	41.9	---

[a]See reference 24. [b]See reference 25. [c]See reference 26.

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it has the relative energy correct (RDX less than HMX). Improvement in
this area may be possible, but the project objective for MM2 was to
achieve accurate geometries and correct relative energies, which has
been done.

Conclusions

The program MM2 has been parameterized to allow calculation of
nitramine containing compounds. It can be used to quickly generate a
geometry for any known, or suggested (unsynthesized), compound. The
energies obtained can be used to compare different compounds of
potential use in rocket propellants. The geometries may also be used as
input to other programs (semi-empirical and ab initio) and save a large
amount of computer time normally involved in geometry optimizations.
The final parameters derived for MM2 are shown in Tables 3-5 [Ref 27].

TABLE 3. Bond and dipole parameters developed for nitramine work.

BOND TYPE	K(S)	L(0)	MOMENT
1 - 29	3.750	1.4700	-0.450
7 - 29	9.600	1.2000	-4.500
9 - 29	4.500	1.3300	-0.450
1 - 9	3.400	1.4250	unchanged

TABLE 4. Bond angle (bending) parameters developed for nitramine work.

ATOM TYPES			K(B)	THETA(0)	ED. TYPE
7	29	7	3.000	125.000	
	29	1	0.612		
1	29	7	3.500	118.000	
	29	7	0.612		
7	29	9	3.500	118.000	
	29	9	0.612		
1	9	29	2.460	117.000	
	9	29	0.000		

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TABLE 4 (continued)

ATOM TYPES			K(B)	THETA(O)	ED. TYPE
1	9	1	2.460	124.000	
	9	1	0.000		
9	1	9	1.450	109.470	1
9	1	9	1.450	109.510	2
9	1	9	1.450	109.500	3
9	1	5	0.360	109.390	1
9	1	5	0.360	109.410	2
9	1	5	0.360	110.000	3
1	1	29	0.570	109.470	1
1	1	29	0.570	108.800	2
1	1	29	0.570	109.500	3
29	1	29	1.600	104.000	
1	1	9	0.570	109.470	1
1	1	9	0.570	108.800	2
1	1	9	0.570	109.500	3
29	1	11	0.560	107.500	
11	1	29	0.560	107.500	

TABLE 5. Torsional parameters developed for nitramine work.

ATOM TYPE NOS.				V1	V2	V3
1	9	29	7	0.000	1.200	0.000
9	1	9	29	0.000	0.000	0.350
5	1	9	29	0.000	0.000	0.520
1	1	1	29	0.170	0.270	0.093
5	1	1	29	0.000	0.000	0.500
1	1	29	7	-0.300	1.200	-0.350
5	1	29	7	-0.167	0.000	-0.100
1	9	1	9	0.000	0.000	0.350
9	1	9	1	0.000	0.000	0.350
9	1	1	1	0.000	0.000	0.000
1	9	1	5	0.000	0.000	0.520
1	1	9	1	-0.200	0.730	0.800
1	9	1	1	-0.200	0.730	0.800
9	1	1	29	-0.400	-1.100	1.200
1	1	9	29	0.000	1.200	-0.350
9	1	1	11	0.000	0.500	0.250
29	1	29	7	0.000	0.000	0.350
7	29	1	11	0.000	1.000	0.350
9	1	1	9	2.100	0.270	0.093
9	1	1	5	0.000	0.000	0.500

QUANTUM MECHANICS THEORETICAL BACKGROUND

The tenets of quantum mechanics [quantum texts] state that the energy and many properties of a stationary state of a molecule can be obtained by the solution of the Schrödinger equation [Ref. 28] below.

$$H\Psi = E\Psi \qquad\qquad (4)$$

Here H is the Hamiltonian, the energy operator; E is the numerical value of the energy of the state as compared to the energy of all particles of the molecule separated at infinite distance; and Ψ is the wavefunction of the molecule. The square of the wavefunction can be interpreted as the probability distribution of the particles within the molecule. The Hamiltonian may be separated into kinetic and potential energy terms. The potential energy terms may be further separated into such energy terms as the electronic, nuclear, spin and spin-orbit Hamiltonians.

The solution for the wave equation is too complex to solve exactly for all molecules except the H_2^+ species. In order to allow for any further calculations certain assumptions must be made. The most important assumption is the Born-Oppenheimer approximation [Ref. 29] which states that the motion of the electronic and nuclear portions of the molecule can be separated. This is based on the assumption that the difference in masses of the nuclei and electrons is sufficient to cause a substantial difference in the velocities of the two particles. The result is that the nucleus can be assumed to be stationary in comparison to electron movement. This reduces the problem to the calculation of

electron motion in a stationary field of fixed nuclei. The energy term for the nuclear portion of the Hamiltonian is fixed for a set geometry and is readily calculated.

The main task then of most theoretical studies is to solve the electronic Schrödinger equation by finding the appropriate wave function for a set geometry of nuclei and determine the energy. Each geometric parameter may be varied and the energies recalculated. These values may be plotted to produce a potential energy surface (or curve in the case of a diatomic). The low point on the surface corresponds to an energy minima and is considered the low energy configuration of the molecule. There may be other stationary points on the surface, such as an energy peak, which corresponds to a transition state, or a saddle point, which is where there are one or more orthogonal directions in which the energy is at a maximum.

The most common approach to solving the Schrödinger equation and developing the appropriate wave functions is to employ molecular orbital theory. Here the wave functions are approximated by one-electron functions or orbitals. These orbitals are combined to approximate the full molecular wave function.

Molecular Orbital (MO) Theory

The object of all molecular orbital (MO) calculations is to build a set of molecular orbitals to be occupied by the electrons contained within the molecule. Most MO calculations employ the linear combination of atomic orbitals (LCAO) formalism to accomplish this. The LCAO method builds the molecular orbitals from the atomic orbitals (AOs) centered on the constituent atoms. The MO calculation involves finding the

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combinations of these atomic orbitals that have the proper symmetries and that give the lowest electronic energy.

The construction of good SCF MOs (LCAO method) depends on having a well-chosen basis set. Finite linear combinations of basis functions can then be used to approximate atomic orbitals to the desired level of accuracy within the limits of the computer. Basis sets used in accurate computations of molecular wave functions are usually best set up by first adopting optimum basis sets previously obtained for the respective atoms and adding polarization (diffuse) functions. Polarization functions have higher azimuthal quantum numbers than the occupied orbitals for the respective atoms [Ref. 30 and 31] or are functions centered in regions of space other than at the atoms [Ref. 32]. Good atomic basis sets and polarization functions are available from the literature. [There are many published basis set collections. For a representative collection, see Refs. 33-35.]

The simplest example is that of the hydrogen molecule. Hydrogen's molecular orbitals results from the combination of two hydrogen 1s atomic orbitals. The symmetry properties of these orbitals require that all symmetry species must be either symmetric or antisymmetric with respect to a mirror plane midway between the two atoms and perpendicular to the connecting line between them. Only two types of atomic orbital combinations fulfill these requirements. The two in-phase or symmetric atomic orbitals can be added, forming a symmetrical molecular orbital or bonding combination. If the two atomic orbitals are out of phase they produce an antisymmetric antibonding combination. When two electrons are added they occupy the lowest energy molecular orbital, which in this case is the bonding orbital resulting in a stable hydrogen molecule.

The higher energy orbital is unoccupied. This virtual orbital therefore makes no contribution to the molecule's electronic energy. The magnitude of the coefficients of the atomic orbitals is determined by the normalization procedure, and express the contribution of each orbital to the eventual molecular orbital. This arises from the fact that the probability of finding an electron in the molecular orbital must be equal to one. In the case of the hydrogen molecule, the coefficients are equal due to the symmetry of the species, but this is not always the case. Indeed, much of the effort in determining the lowest energy molecular orbital involves determining the correct coefficient for each atomic orbital. The energy of an electron in a molecular orbital is determined by bonding interactions, or overlap, between two atomic orbitals and the electron's energy in the isolated atomic orbital. The lowest energy molecular orbital is a compromise between the need to maximize the atomic orbital overlap (when the coefficients are equal) and the tendency for the electrons to occupy the most stable atomic orbital. Therefore, the greater the energy difference between two atomic orbitals, the more unsymmetrical will be the bonding molecular orbital. The coefficients can be used to obtain a 'population analysis' which indicates the electron distribution and charge on each atom.

An additional interaction must be considered when performing highly accurate calculations. An electron in a molecular orbital is also influenced by the other electrons within a molecule. This electron-electron repulsion is generally taken into account in MO calculations by consideration of the interactions between a single electron in a given molecular orbital and a mean field produced by all

the other electrons within a molecule. This approach is known as the self-consistent field (SCF) method, and is generally an iterative procedure in which the orbitals are improved from cycle to cycle until electronic energy reaches a constant minimum and the orbitals no longer change. This situation is known as "self consistent." SCF calculations are also known as Hartree-Fock or single-determinant theory.

SCF calculations usually overestimate the electron-electron repulsion contribution. This is because the theory does not allow the electrons to avoid one another. It assumes the electron positions are independent of one another. The error introduced is reasonably quite consistent so that it's effects can be minimized, particularly if proper comparisons are made. For example, the determination of stabilization energy can be made fairly accurately if the equation involved is isodesmic.

In reality electron positions are not independent of each other. If there are two electrons in an orbital, they will tend to stay apart, minimizing the electron repulsion energy. Computational methods to handle such effects are known as electron correlation methods. Computational procedures such as the multiconfiguration-SCF and configuration interaction methods are available for such purposes within many ab initio programs.

Another difficulty in MO calculations is the treatment of open shell and closed shell·systems. Closed shell systems are almost always calculated with restricted Hartree-Fock (RHF) theory. In RHF methods the molecular orbitals are calculated, but each orbital is restricted to be doubly occupied. With this restriction electron spin problems do not occur since all the electrons are paired. In open shell systems, where

there is an unpaired electron, the electron spin factors play a role and comparisons at the same level of approximations become difficult. One way to treat the problem is to perform Unrestricted Hartree-Fock (UHF) calculations. In this formalism two sets of orbitals are calculated (commonly labeled alpha and beta), one for each type of spin. In general, UHF and RHF results should not be compared.

Molecular Orbital Computational Procedures

The computational process may be summarized by the following steps [Ref. 36]:

1) Specify a set of atomic orbitals (the basis set). Normally Gaussian orbitals

$$\chi_{nlm}(r) = Nr^{n-1}\exp(-\alpha r^2)Y_{lm}(\Theta, \phi) \tag{5}$$

are used which are converted into real form by appropriate linear combinations (r is the orbital radius, nlm are the quantum numbers, N is a normalization constant, $\exp(-\alpha r^2)$ is the gaussian component, and Y is the angular function of the orbital).

2) Compute the overlap integrals

$$S_{\mu\nu} = \int \phi_\mu^*(1)\phi_\nu(1)d\tau_1 \tag{6}$$

of orbitals ϕ_μ and ϕ_ν on atom 1 over the space of atom 1.

3) Compute the core Hamiltonian matrix

$$H_{\mu\nu} = \int \phi_\mu(1)H_o(1)\phi_\nu(1)d\tau_1 \tag{7}$$

where H_o is the core Hamiltonian operator.

4) Compute the two-electron integrals

$$\langle \mu\nu|\lambda\sigma\rangle = \int \phi_\mu(1)\phi_\nu(1)(e^2/r_{12})\phi_\sigma(2)\phi_\lambda(2)d\tau_1 d\tau_2 \tag{8}$$

where r_{12} is the internuclear separation.

5) Compute the eigenvectors of $H_{\mu\nu}$. This gives a starting set of LCAO coefficients (and the initial set of molecular orbitals).

6) Assign electrons in pairs to the lowest molecular orbitals until all the electrons have been assigned.

7) Compute the density matrix

$$P_{\mu\nu} = 2\sum_i^{occ} c^*_{\mu i}c_{\nu i} \tag{9}$$

where the c's are the coefficients of orbitals μ and ν in the LCAO approximation. A factor of 2 appears because of the double occupancy of the MO by two electrons of opposite spin (occ = occupied).

8) Compute the total electronic energy.

$$E = \sum_{\mu\nu}P_{\mu\nu}H_{\mu\nu} + \tfrac{1}{2}\sum_{\mu\nu\lambda\sigma}P_{\mu\nu}P_{\lambda\sigma}[\langle\mu\nu|\lambda\sigma\rangle - \tfrac{1}{2}\langle\mu\lambda|\nu\sigma\rangle] \tag{10}$$

9) Compute the Fock Hamiltonian.

$$F_{\mu\nu} = H_{\mu\nu} + \sum_{\lambda\sigma}P_{\lambda\sigma}[\langle\mu\nu|\lambda\sigma\rangle - \tfrac{1}{2}\langle\mu\lambda|\nu\sigma\rangle] \tag{11}$$

10) Compute the eigenvectors of $F_{\mu\nu}$ to obtain a second set of LCAO coefficients.

11) Continue until the total energy E remains constant to the required accuracy (self-consistent).

AB INITIO (GAUSSIAN 82 AND GAMESS)

As a result of this project two ab initio molecular orbital computational programs are available for general use at the AFAL. Those two are Gaussian 82 and GAMESS. A third, Gaussian 76 [Ref. 37], was also installed but has been supplanted by the newer revised version of the Gaussian series, Gaussian 82. A fourth program, HONDO 5 [Ref. 38], was obtained to run on the CDC. Unfortunately, it would not operate properly on the CDC hardware installed at the AFAL. Both Gaussian 82 and GAMESS run on the VAX cluster. In addition GAMESS is able to run on the FPS. Both programs are widely used within the chemistry community and are installed at a large number of computer sites. A brief description of each program's history and capabilities follows, along with a sample input and output examples.

Gaussian 82 Program Description

Gaussian 82 is the latest of a series of programs designed to perform ab initio molecular orbital calculations. The first, Gaussian 70, has evolved through Gaussian 76, Gaussian 80, and finally to the current Gaussian 82 (Gaussian 87 is expected to be available soon). This series of programs is largely the product of Professor John Pople, at Carnegie-Mellon University, and Professor Warren J. Hehre at the University of California, Irvine, and their respective research groups. Gaussian 82 is a connected series of programs that perform the ab initio calculations and have been implemented on VAX/VMS, Cray/COS, Cray/CTSS, and IBM/MVS computers and operating systems. The earlier versions of the program can be obtained from the Quantum Chemistry Program Exchange

at Indiana University. The latest versions may be obtained directly from Dr Pople at Carnegie-Mellon.

Gaussian 82 has been designed to be user friendly as much as possible. All standard input is in free-format and the commands all use keywords as opposed to numerical codes. The output is generally self-explanatory. The default values can be overridden for more advanced use, though the default values are generally very reasonable. As a result of its ease of use and wide spread availability, Gaussian 82 has become the most widely used ab initio computational tool.

Capabilities of the Gaussian 82 program include [Ref. 39]:

- Calculation of one and two electron integrals over s, p, d, and f contracted gaussian functions employing a variety of stored basis sets.

- Self-consistent field calculations for restricted closed-shell (RHF) and open shell restricted Hartree-Fock wavefunctions (ROHF).

- Evaluation of various one-electron properties of the Hartree-Fock wavefunction, including Mulliken population analysis and electrostatic fields.

- Automated geometry optimization to either minima or saddle points, and for numerical differentiation to produce force constants.

- Correlation energy calculations using Moller-Plesset perturbation theory carried out to second, third, or fourth order. (MP2, MP3, MP4)

- Correlation energy calculations using configuration interaction

with either all double excitation or all single and double excitations. (CI, CID, CISD)

- Correlation energy calculations using coupled cluster theory with double substitutions. (CCD)
- Computation of force constants (nuclear coordinate second derivatives) analytically for RHF and UHF energies and numerically for RHF, UHF, MP2, CID, and UCISD energies.
- Testing the SCF wave function for stability under release of constraints.

One drawback to Gaussian 82 is that it does not include MCSCF capabilities. MCSCF becomes most necessary when calculating excited states because there are many excited configurations that should be included when formulating the wavefunction. As a result Gaussian 82 is basically restricted to ground state systems.

Installation of Gaussian 82

The Gaussian 82 system of programs was installed very easily. VAX command files were included on the distribution tape to handle compilation and linking. Several important modifications on the VAX were necessary. First, all users of the program must have two privileges, GRPNAM and PRMCEB. These privileges allow Gaussian 82 to establish unique process and file names. The program utilizes the user's group account number in the file and process names. However, for users in the same group account, there will be duplication. The PRMCEB privilege allows access to a common event flag cluster containing 10 flags (0-9). Each number can only be used by one job at a time, so this provides the

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true uniqueness in the process and file names. The GRPNAM privilege allows a user to place some of the Gaussian 82 logical names in a table accessible by other members of the group account. This is another way to prevent name duplication.

GAMESS Program Description

GAMESS was originally assembled by the staff of the National Resource for Computational Chemistry in 1980. [Ref. 40]. The continued development over the past few years has largely been through the efforts of Professor M. S. Gordon at North Dakota State University, and Pro- fessor K. Ruedenberg at Iowa State University and their research groups. GAMESS is a synthesis of many different programs, with a large part coming from the older HONDO programs. The VAX version of GAMESS installed at AFAL was obtained from Dr Gordon at North Dakota State University, and the FPS version was obtained from Dr Steve Elbert at Iowa State University.

GAMESS offers a wide range of quantum chemical calculations including [Ref. 41]:

- RHF SCF molecular wave functions (Restricted Hartree Fock)

- UHF SCF molecular wave functions (Unrestricted Hartree Fock)

- ROHF SCF molecular wave functions (Restricted Open Shell Hartree Fock)

- GVB SCF molecular wave functions (Generalized Valence Bond)

- MCSCF SCF molecular wave functions (Multi-Configuration SCF)

- CI SCF molecular wave functions (Configuration Interaction)

- Performs molecular geometry optimization using energy gradients

in terms of Cartesian or internal coordinates.

- Searches for potential energy saddle points.

- Traces intrinsic reaction path from a saddle point to reactants or products.

- Computes normal modes and vibrational frequencies.

- Calculates the the following properties:

    - dipole, quadrupole, and octapole moments

    - electrostatic potentials

    - electric field and electric field gradients

    - electron density and spin density

    - Mulliken and Lowdin population analysis

    - localized orbitals by the Boys method

    - virial theorem and energy components

The program is limited to a total of 50 atoms; the total number of symmetry unique shells cannot exceed 120 shells containing no more than 440 symmetry unique Gaussian primitives. The total number of contracted basis functions cannot exceed 255. Most memory allocations are dynamic within a fixed-length common block. The program checks for CPU time and will stop if time is running short. Restart data are printed and punched out automatically, so the run can be restarted where it left off. In general the program is more difficult to run than Gaussian 82, but it contains more features and control. Since MCSCF procedures are included excited state systems can be calculated.

Installation of GAMESS

GAMESS was also easy to install on both the VAX and FPS. The only

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modification necessary was to the variable in GAMESS telling it how much memory is available (MEMSIZ). This variable depends on the user's molecular system and the kinds of calculations he will ask GAMESS to perform. If a complex calculation is requested (e.g. in MCSCF) on a system with a large number of electrons (e.g. XeO), then another problem may arise. Even if the program thinks it has enough memory, it may be using a large amount of the virtual memory on the VAX. Virtual memory is actually a file on disk which is initialized on system startup. Memory addressing continues from physical memory to disk. A computation will be drastically hampered if an insufficient amount of physical memory has been allocated. The flag to watch for in this situation is the amount of paging the job does. Paging is when a section of memory is temporarily written to disk to allow another part of the program to execute. Excessive paging (a large number of page faults) will decrease utilization of the computer, since the computation will constantly be waiting on the paging I/O to disk. This problem has been overcome by increasing the amount of physical memory available to jobs running in selected batch queues.

Each of these programs was fairly easy to install. Execution is facilitated by the use of command files to handle job control and I/O. Examples of the command files used for each of these programs are included in Appendix B.

Results

The objective of the project was to install and make useful certain computational tools that will benefit the research chemist. In terms of

the ab initio programs there was little to do in the way of modification or parametrization of the programs themselves due to the nature of the ab initio method. Indeed, the only input to the programs, besides the description of the molecular system of interest, is a basis set describing the initial atomic orbitals. The use of an accurate basis set is vital to the production of reliable results. Much of the research going on in molecular orbital calculations is centered on the development of improved basis sets. Fortunately both Gaussian 82 and GAMESS include several different basis sets that can be used. In addition, both allow alternate basis sets to be input and used.

Certain test molecules were computed to obtain a comparison to literature values. These comparisons serve to insure the validity of the computations being performed by the installed programs at the AFAL. These test cases showed the programs to be operating without problems. In addition certain molecular systems relating to ongoing work at the AFAL were also computed. One such molecule, nitramide, will be used as the example for the discussion of input and output files.

Gaussian 82 Example

The input file to Gaussian 82 is actually a command (COM) file which executes the program. As seen in the example below Gaussian 82 allows the placement of the files to different disk locations and subdirectories. The files that Gaussian 82 allows the placement of are the %CHK file, which contains restart information, the %RWF file, containing the read/write information for various housekeeping purposes within the program, and %INT file, which contains the one and two electron integral files. The control line starts with a '#' and

contains list directed one word directives for the program. This line

instructs the program as to what type of SCF calculation to do; what

basis set to use; whether to do an optimization, transition state, or

frequency calculation; which electron correlation techniques to use if

any; what kind of information is to be printed; and other such controls

for the calculation.

```
ASSIGN USER$DISK11:[SCRATCH.DISK11] GAUSS_SCRDIR
$ RunGauss
%CHK=USER$DISK5:[RODGERSS]NITRAAMIDE631STAR.CHK
%RWF=USER$DISK5:[RODGERSS]NITRAMIDE631STAR.RWF
%INT=USER$DISK5:[RODGERSS]NITRAMIDE631STAR.2ER

# rhf 6-31G* OPT=NOEIGENTEST  minpop

G82 NITRAMIDE

0 1
    H
    N  1  1.017799
    N  2  NN       1  NNH
    O  3  1.209101 2  ONN      1  dihed
    O  3  1.209101 2  ONN      1  dihed1
    H  2  1.017799 3  NNH      5  HNNO

NN= 1.3519
dihed=23.6959
dihed1=200.954
ONN=116.66633
NNH=110.2873
HNNO=33.0
```

The next line is simply a title or identifying description of the

calculation. The charge and multiplicity of the molecule is next

specified followed by the Z-matrix specifying the molecules connectivity

and internal parameters (bond lengths, bond angles, torsion angles). If

any of these parameters are to be fixed the numerical value may be

input. If the parameter is to be optimized then a variable name can be

input with its initial value listed below the matrix. If there are two

blank lines following the matrix then the values are assumed to be fixed

by the program and they are not optimized. A large number of options

are available to control the calculation and are described quite well in

the accompanying users manual [Ref. 39]. The Gaussian 82 output is also

described well in the manual and also in "A Handbook of Computational

Chemistry" [Ref. 19]. The type of output information is very similar to

that of GAMESS, described in more detail below.

GAMESS Examples

The following is a GAMESS input example to calculate the SCF

wave function and energy of nitramide with a 6-31G basis set and

polarization functions on the second row elements. The input is

initiated with a control section which contains the global control

parameters such as multiplicity, charge, type of SCF calculation to be

performed, the run type, and the amount of information to be printed.

Different sections can then be added to control specific types of

calculations. In this case the SIGX group controls the geometry search

conditions. Geometry optimizations and transition state searches can be

performed using cartesian coordinates or by employing internal coor-

dinates. The ZMAT group sets up the molecules internal coordinates to

perform the geometry optimization. Next follows a DATA group where the

actual molecule and its initial geometry is specified. Here the basis

set is determined and any polarization functions are added. A more

detailed list of the parameters and description of the input file can be

found in the GAMESS manual.

```
$CONTRL  SCFTYP=RHF   MULT=1 NPRINT=-6 RUNTYP=OPTIMIZE
 TIMLIM=15000  MAXIT=40 UNITS=BOHR  NZVAR=12 $END
$SIGX NSTEP=140 $END
$ZMAT IZMAT(1)=1,1,3, 1,2,3, 1,3,4, 1,4,6,1,4,5,
2,1,3,2,2,5,4,6,2,3,4,5, 2,3,4,6, 2,1,3,4, 2,2,3,4, 3,1,3,4,6  $END
 $DATA
NITRAMIDE 631G* BASIS SET
C1
HYDROGEN    1.0   0.5154832        0.4844269         -0.0566758
    1        6  N31


HYDROGEN    1.0  -0.7662438        1.7169845          2.6165991
    1        6  N31


NITROGEN    7.0   0.1673385        0.3046024          1 7871923
    1        6  N31
    2    D   1
    1        0.8            1.0


NITROGEN    7.0   2.3290509       -0.2145173          3.0627199
    1        6  N31
    2    D   1
    1        0.8            1 0


OXYGEN      8.0   3.9656336       -1.2251145          1.8945165
    1        6  N31
    2    D   1
    1        0.8            1.0


OXYGEN      8.0   2.3585770        0.3219516          5.2479824
    1        6  N31
    2    D   1
    1        0.8            1.0


 $END
```

Selected sections of the output from this nitramide run are shown
below. The command file to run the program sets system parameters and
then makes file assignments. These files will be used for storage of
the electron integrals, the restart data, wave function vectors, and
various other information needed by the program. This particular run
was performed on the AFAL FPS and the next lines seen are the FPS Job
Control Language (JCL). The program is then initiated and executed.
The input file is read and reprinted in the output file.

```
$ V = F$VERIFY(0)      ! turn off command verification in SYLOGIN.COM
$ EXIT                 ! exiting SYLOGIN.COM command file
$!   COMMAND FILE TO RUN AN FPS GAMESS JOB. THIS FILE SHOULD RESIDE IN
THE
$!   GAMESS DIRECTORY. IT SHOULD BE ACCESSED FROM GAMESS.COM, BUT CAN
$!   STAND ALONE, IF NECESSARY.
$!
$!   THE CALL IS        $RGAMESS_FPS filename  directory
$!
$    SHOW TIME
   7-MAY-1987 08:52:59
$!
$    SET VERIFY
$ ON ERROR THEN GOTO AA
$ ON CONTROL_Y THEN GOTO AA
$!
$!   Make assignments
$!
$    IF P2 .NES. ""    THEN SET DEFAULT
USER$DISK1:[RODGERSS.GAMESSHOME]
$ assign user$disk11:[scratch.fps_scratch] scr
$ NAME = F$EXT(0,15,P1)
$ SET PROCESS/NAME=NITR
$ COPY NITR.INP SCR:NITR.F05   ! Pick up the input data
$ ASSIGN SCR:NITR.IRC   IRCDATA
$ ASSIGN SCR:NITR.F05   INPUT
$ ASSIGN SYS$OUTPUT     OUTPUT
$ ASSIGN SCR:NITR.DAT   PUNCH
$ ASSIGN SCR:NITR.F08   INTGRLS
$ ASSIGN SCR:NITR.F09   ORDINT
$ ASSIGN SCR:NITR.F09   JKFILE
$ ASSIGN SCR:NITR.F10   DICTNRY
$ ASSIGN SCR:NITR.F11   DRTFILE
$ ASSIGN SCR:NITR.F12   CIVECTR
$ ASSIGN SCR:NITR.F15   WORK15
$ ASSIGN SCR:NITR.F16   WORK16
$ ASSIGN SCR:NITR.F20   DASORT
$!
$! Go to the FPS
$!
$ SJE/TIME/CONTINUE
SJE-I-WELCOME, SJE REL F03-200  VER 1.0      05/07/87  08:53.
      ATTACH/WAIT/TMRAM
APEX-I-SUMREL, The SUM currently executing is: F03-000.
SJE-I-ATTACH,08:53:12, Assigned AP number  1, priority= 1, jobnum=  17.
      COPYIN INPUT,INPUT
SJE-I-COPYIN,08:53:15, File copied in.
      COPYIN/B USER$DISK1:[G82.GAMESS]GAMES.IMG,GAMESS
SJE-I-COPYIN,08:53:33, File copied in.
      DIR
Directory = ():SCRATCH16():
   GAMESS                          INPUT
      CLEAR/ALL
      SHOW/CPU
```

CPU Usage: 0.0669 seconds

        GAMESS

****
*   *
* GAMESS VERSION 1.02 - REVISION 1 OCT 80 - QG01.2   *
* NRCC STAFF - M.DUPUIS, D.SPANGLER, J.WENDOLOSKI   *
*   NORTH DAKOTA STATE UNIVERSITY AND IOWA STATE UNIVERSITY*
* - M. SCHMIDT, S. ELBERT   *
*   REVISION 30 NOV 1986   *
*   *
*************************** VERSION **********************

EXECUTION OF GAMESS BEGUN 7-MAY-1987 08:53:52

 1250000 WORDS REQUESTED 1396736 WORDS AVAILABLE   146736 WORDS REMAIN FREE

            ECHO OF THE FIRST FEW INPUT CARDS -
INPUT CARD> $CONTRL SCFTYP=RHF   MULT=1 NPRINT=-6 RUNTYP=OPTIMIZE
INPUT CARD> TIMLIM=15000 MAXIT=40 UNITS=BOHR NZVAR=12 $END
INPUT CARD> $SIGX NSTEP=140 $END
INPUT CARD> $ZMAT IZMAT(1)=1,1,3, 1,2,3, 1,3,4, 1,4,6, 1,4,5, 2,1,3,2,
INPUT CARD> 2,5,4,6,2,3,4,5, 2,3,4,6, 2,1,3,4, 2,2,3,4, 3,1,3,4,6$END
INPUT CARD> $DATA
INPUT CARD>NITRAMIDE 631G* BASIS SET
INPUT CARD>C1
INPUT CARD>HYDROGEN   1.0   0.5154832   0.4844269   -0.0566758
INPUT CARD>   1   6   N31
INPUT CARD>
INPUT CARD>HYDROGEN   1.0 -0.7662438   1.7169845   2.6165991
INPUT CARD>   1   6   N31
INPUT CARD>
INPUT CARD>NITROGEN   7.0   0.1673385   0.3046024   1.7871923
INPUT CARD>   1   6   N31
INPUT CARD>   2   D   1
INPUT CARD>   1   0.8   1.0
INPUT CARD>
INPUT CARD>NITROGEN   7.0   2.3290509   -0.2145173   3.0627199
INPUT CARD>   1   6   N31
INPUT CARD>   2   D   1
INPUT CARD>   1   0.8   1.0
INPUT CARD>
INPUT CARD>OXYGEN   8.0   3.9656336   -1.2251145   1.8945165
INPUT CARD>   1   6   N31
INPUT CARD>   2   D   1
INPUT CARD>   1   0.8   1.0
INPUT CARD>
INPUT CARD>OXYGEN   8.0   2.3585770   0.3219516   5.2479824
INPUT CARD>   1   6   N31
INPUT CARD>   2   D   1
INPUT CARD>   1   0.8   1.0
INPUT CARD>
INPUT CARD> $END

The next portion of the program prints the information and options the input file has provided. This provides an easy way to insure that the desired selections have been made. This section of the output file also lists the basis sets that will be used in the computation. The number of molecular shells, electrons, multiplicity, and occupied and unoccupied orbitals are then listed, followed by the job options for the run.

```
**************************************************************
*                                                            *
*      NITRAMIDE 631G* BASIS SET                             *
*                                                            *
**************************************************************
```

THE POINT GROUP OF THE MOLECULE IS ...C1
THE ORDER OF THE PRINCIPAL AXIS IS ...   0

```
                      *******************
```

MOLECULAR BASIS SET

```
                      *******************
```

THE CONTRACTED PRIMITIVE FUNCTIONS HAVE BEEN UNNORMALIZED
THE CONTRACTED BASIS FUNCTIONS ARE NOW NORMALIZED TO UNITY

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
```

ATOM	ATOMIC	COORDINATES (BOHR)		
	CHARGE	X	Y	Z

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
```

* HYDROGEN	1.0	0.5154832000	0.4844269000	−0.0566758000 *
* HYDROGEN	1.0	−0.7662438000	1.7169845000	2.6165991000 *
* NITROGEN	7.0	0.1673385000	0.3046024000	1.7871923000 *
* NITROGEN	7.0	2.3290509000	−0.2145173000	3.0627199000 *
* OXYGEN	8.0	3.9656336000	−1.2251145000	1.8945165000 *
* OXYGEN	8.0	2.3585770000	0.3219516000	5.2479824000 *

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
```

ATOMIC BASIS SET

SHELL	TYPE	PRIM	EXPONENT	CONTRACTION COEFFICIENTS			

HYDROGEN

1	S	1	18.731137	0.214935	(0.033495)		
1	S	2	2.825394	0.364571	(0.234727)		
1	S	3	0.640122	0.415051	(0.813757)		
2	S	4	0.161278	0.181381	(1.000000)		

HYDROGEN

3	S	5	18.731137	0.214935	(0.033495)		
3	S	6	2.825394	0.364571	(0.234727)		
3	S	7	0.640122	0.415051	(0.813757)		
4	S	8	0.161278	0.181381	(1.000000)		

NITROGEN

5	S	9	4173.511460	0.678998	(0.001835)		
5	S	10	627.457911	1.250431	(0.013995)		
5	S	11	142.902093	2.020356	(0.068587)		
5	S	12	40.234329	2.644212	(0.232241)		
5	S	13	12.820213	2.265005	(0.469070)		
5	S	14	4.390437	0.779188	(0.360455)		
6	L	15	11.626362	-0.515875	(-0.114961)	2.068052	(0.067580)
6	L	16	2.716280	-0.255023	(-0.169117)	1.610011	(0.323907)
6	L	17	0.772218	0.672735	(1.145852)	0.764490	(0.740895)
7	L	18	0.212031	0.222695	(1.000000)	0.205088	(1.000000)
8	D	19	0.800000	1.113825	(1.000000)		

NITROGEN

9	S	20	4173.511460	0.678998	(0.001835)		
9	S	21	627.457911	1.250431	(0.013995)		
9	S	22	142.902093	2.020356	(0.068587)		
9	S	23	40.234329	2.644212	(0.232241)		
9	S	24	12.820213	2.265005	(0.469070)		
9	S	25	4.390437	0.779188	(0.360455)		
10	L	26	11.626362	-0.515875	(-0.114961)	2.068052	(0.067580)
10	L	27	2.716280	-0.255023	(-0.169117)	1.610011	(0.323907)
10	L	28	0.772218	0.672735	(1.145852)	0.764490	(0.740895)
11	L	29	0.212031	0.222695	(1.000000)	0.205088	(1.000000)
12	D	30	0.800000	1.113825	(1.000000)		

OXYGEN

13	S	31	5484.671660	0.831724	(0.001831)		
13	S	32	825.234946	1.530816	(0.013950)		
13	S	33	188.046958	2.477149	(0.068445)		
13	S	34	52.964500	3.256281	(0.232714)		
13	S	35	16.897570	2.792893	(0.470193)		
13	S	36	5.799635	0.954938	(0.358521)		
14	L	37	15.539616	-0.617934	(-0.110778)	3.116944	(0.070874)
14	L	38	3.599934	-0.275721	(-0.148026)	2.401438	(0.339753)
14	L	39	1.013762	0.814208	(1.130767)	1.054360	(0.727159)
15	L	40	0.270006	0 266956	(1.000000)	0.277432	(1 000000)
16	D	41	0 800000	1 113825	(1.000000)		

OXYGEN

17	S	42	5484.671660	0.831724	(0.001831)		
17	S	43	825.234946	1.530816	(0.013950)		
17	S	44	188.046958	2.477149	(0.068445)		
17	S	45	52.964500	3 256281	(0.232714)		
17	S	46	16.897570	2.792893	(0.470193)		
17	S	47	5.799635	0.954938	(0.358521)		
18	L	48	15.539616	-0.617934	(-0.110778)	3.116944	(0.070874)
18	L	49	3.599934	-0.275721	(-0.148026)	2.401438	(0.339753)
18	L	50	1.013762	0.814208	(1.130767)	1.054360	(0.727159)
19	L	51	0.270006	0.266956	(1.000000)	0.277432	(1.000000)
20	D	52	0.800000	1.113825	(1.000000)		

TOTAL NUMBER OF SHELLS   = 20

TOTAL NUMBER OF BASIS FUNCTIONS   = 64

NUMBER OF ELECTRONS   = 32

CHARGE OF MOLECULE   = 0

STATE MULTIPLICITY   = 1

NUMBER OF OCCUPIED ORBITALS (ALPHA) = 16

NUMBER OF OCCUPIED ORBITALS (BETA) =   16

TOTAL NUMBER OF ATOMS   = 6

THE NUCLEAR-NUCLEAR REPULSION ENERGY IS   130.2207714621

JOB OPTIONS

SCFTYP=RHF		RUNTYP=OPTIMIZE	ICHARG=	0
MULT =	1	UNITS =BOHR	TIMLIM=	900000.0
INTTYP=POPLE		LOCAL =NONE	MAXIT =	40
NPRINT=	-6	IREST =	0	OPTTOL=	0.000500
IOPTRD=	0	NORMF =	0	NORMP =	0
ITOL =	20	ICUT =	9	NZVAR =	12
NOSYM =	0	LIGSW =	1	IOVLP =	0
GEOM =INPUT				

The next section displays the geometrical description of the molecule in terms of a Z-matrix. A Z-matrix consists of the bond lengths, bond angles, and torsion angles within the molecule. Not every parameter needs to specified, only those which are necessary to completely describe the molecule. Normally 3N-6 parameters (3N-5 for linear molecules), where N is the number of atoms, are required to be entered. GAMESS employs a coded Z-matrix where the type is specified by a numerical code. Bond lengths are 1, bond angles are 2, and torsion angles are 3. GAMESS uses the Z-matrix for geometry optimizations, transition state and intrinsic reaction coordinates searches, and to fix certain parameters. The Cartesian coordinates are still required for the initial input, unlike Gaussian 82. The output will display the Z-matrix and then the value of each parameter. It will also display interatomic distances derived from the Cartesian coordinates.

```
         —— CODED Z MATRIX INPUT ——
    COORD   TYPE    I   J   K   L   M
      1      1      1   3
      2      1      2   3
      3      1      3   4
      4      1      4   6
      5      1      4   5
      6      2      1   3   2
      7      2      5   4   6
      8      2      3   4   5
      9      2      3   4   6
     10      2      1   3   4
     11      2      2   3   4
     12      3      1   3   4   6
```

INTERNAL COORDINATES

NO.	TYPE	I	J	K	L	M	COORDINATE (BOHR,RAD)	COORDINATE (ANG,DEG)
1	STRETCH	1	3				1.8850441	0.9975222
2	STRETCH	2	3				1.8852890	0.9976519
3	STRETCH	3	4				2.5630951	1.3563314
4	STRETCH	4	6				2.2503428	1.1908300
5	STRETCH	4	5				2.2504241	1.1908730
6	BEND	1	3	2			2.0379158	116.7639732
7	BEND	5	4	6			2.2163051	126.9849278
8	BEND	3	4	5			2.0330518	116.4852895
9	BEND	3	4	6			2.0331341	116.4900018
10	BEND	1	3	4			1.9287265	110.5078862
11	BEND	2	3	4			1.9288401	110.5143958
12	TORSION	1	3	4	6		2.7304730	156.4445776

INTERNUCLEAR DISTANCES (ANGS.)

		HYDROGEN	HYDROGEN	NITROGEN	NITROGEN	OXYGEN	OXYGEN
1	HYDROGEN	0.0000000	1.6990148	0.9975222	1.9449100	2.2842575	2.9729581
2	HYDROGEN	1.6990148	0.0000000	0.9976519	1.9450822	2.9732040	2.2843542
3	NITROGEN	0.9975222	0.9976519	0.0000000	1.3563314	2.1675989	2.1676181
4	NITROGEN	1.9449100	1.9450822	1.3563314	0.0000000	1.1908730	1.1908300
5	OXYGEN	2.2842575	2.9732040	2.1675989	1.19u'730	0.0000000	2.1313281
6	OXYGEN	2.9729581	2.2843542	2.1676181	1.1908300	2.1313281	0.0000000

The calculation is initiated by the formation of the starting molecular orbitals. The program has a facility to make an initial guess at the orbitals or beginning orbitals can be read in. It is these orbitals which will be optimized during the SCF procedure. The more accurate the initial guess is, the faster the computation will proceed.

GUESS OPTIONS

GUESS =HCORE

NORB = 0
NORDER= 0

INITIAL GUESS ORBITALS GENERATED BY HCORE   ROUTINE
..... END OF INITIAL ORBITAL SELECTION ......

STEP CPU TIME = 5.23 TOTAL CPU TIME = 15.79 (0.3 MIN) IS 43.84 PERCENT OF REAL TIME OF 36.02

Next, the program begins the SCF procedure. The output shows how
each option controlling the run is set and then repeats the geometry
data. During the first part of the calculation the one electron and two
electron overlap integrals are calculated. These integrals will be used
throughout the SCF procedure and can be stored for later calculations if
the same basis set is used.

STATIONARY POINT LOCATION RUN		SCHLEGEL METHOD

NNEG	=	0	NFRZ =	0
NSTEP	=	140	IFOLOW =	1
IOPTRD	=	0		
OPTTOL	= 5.000-004		RMIN = 1.500-003	
RMAX	= 1.000-001		RLIM = 7.000-002	
DXMAXT	= 2.000-001		DOTMX = 1.000-002	
UPHESS	=	T	RESTAR =	F

NSERCH= 0

CURRENT NUCLEAR COORDINATES (BOHR)

ATOM	ZNUC	X	Y	Z
HYDROGEN	1.0	0.5154832000	0.4844269000	-0.0566758000
HYDROGEN	1.0	-0.7662438000	1.7169845000	2.6165991000
NITROGEN	7.0	0.1673385000	0.3046024000	1.7871923000
NITROGEN	7.0	2.3290509000	-0.2145173000	3.0627199000
OXYGEN	8.0	3.9656336000	-1.2251145000	1.8945165000
OXYGEN	8.0	2.3585770000	0.3219516000	5.2479824000

INTERNAL COORDINATES

NO.	TYPE	I	J	K	L	M	COORDINATE (BOHR,RAD)	COORDINATE (ANG,DEG)
1	STRETCH	1	3				1.8850441	0.9975222
2	STRETCH	2	3				1.8852890	0.9976519
3	STRETCH	3	4				2.5630951	1.3563314
4	STRETCH	4	6				2.2503428	1.1908300
5	STRETCH	4	5				2.2504241	1.1908730
6	BEND	1	3	2			2.0379158	116.7639732
7	BEND	5	4	6			2.2163051	126.9849278
8	BEND	3	4	5			2.0330518	116.4852895
9	BEND	3	4	6			2.0331341	116.4900018
10	BEND	1	3	4			1.9287265	110.5078862

```
11 BEND      2  3  4            1.9288401    110.5143958
12 TORSION   1  3  4  6         2.7304730    156.4445776
```

               INTERNUCLEAR DISTANCES (ANGS.)
               ─────────────────────────────

		HYDROGEN	HYDROGEN	NITROGEN	NITROGEN	OXYGEN	OXYGEN
1	HYDROGEN	0.0000000	1.6990148	0.9975222	1.9449100	2.2842575	2.9729581
2	HYDROGEN	1.6990148	0.0000000	0.9976519	1.9450822	2.9732040	2.2843542
3	NITROGEN	0.9975222	0.9976519	0.0000000	1.3563314	2.1675989	2.1676181
4	NITROGEN	1.9449100	1.9450822	1.3563314	0.0000000	1.1908730	1.1908300
5	OXYGEN	2.2842575	2.9732040	2.1675989	1.1908730	0.0000000	2.1313281
6	OXYGEN	2.9729581	2.2843542	2.1676181	1.1908300	2.1313281	0.0000000

          ****
          1 ELECTRON INTEGRALS
          ****

...... END OF ONE-ELECTRON INTEGRALS ......

        STEP CPU TIME =   4.63 TOTAL CPU TIME =   20.42 (0.3 MIN) IS 44.36 PERCENT OF REAL
TIME OF   46.03

          ****
          2 ELECTRON INTEGRALS
          ****

THE MAXIMUM NUMBER OF INTEGRALS PER INTEGRAL RECORD = 2725
THE -PK- OPTION IS ON , THE INTEGRALS ARE IN A SUPERMATRIX FORM. -P- AND -K- = F

```
II,JST,KST,LST =   1  1  1  1 NREC =      1 INTLOC =     1 DEL(TIME) =   0.000 TIME =    0.000
II,JST,KST,LST =   2  1  1  1 NREC =      1 INTLOC =     2 DEL(TIME) =   0.007 TIME =    0.007
II,JST,KST,LST =   3  1  1  1 NREC =      1 INTLOC =     7 DEL(TIME) =   0.013 TIME =    0.020
II,JST,KST,LST =   4  1  1  1 NREC =      1 INTLOC =    22 DEL(TIME) =   0.052 TIME =    0.072
II,JST,KST,LST =   5  1  1  1 NREC =      1 INTLOC =    56 DEL(TIME) =   0.067 TIME =    0.139
II,JST,KST,LST =   6  1  1  1 NREC =      1 INTLOC =   121 DEL(TIME) =   0.422 TIME =    0.561
II,JST,KST,LST =   7  1  1  1 NREC =      1 INTLOC =   949 DEL(TIME) =   2.813 TIME =    3.374
II,JST,KST,LST =   8  1  1  1 NREC =      2 INTLOC =   640 DEL(TIME) =   1.941 TIME =    5.315
II,JST,KST,LST =   9  1  1  1 NREC =      5 INTLOC =  1174 DEL(TIME) =   3.933 TIME =    9.248
II,JST,KST,LST =  10  1  1  1 NREC =      6 INTLOC =  2459 DEL(TIME) =   7.014 TIME =   16.261
II,JST,KST,LST =  11  1  1  1 NREC =     15 INTLOC =   842 DEL(TIME) =  17.121 TIME =   33.383
II,JST,KST,LST =  12  1  1  1 NREC =     28 INTLOC =  2153 DEL(TIME) =  10.655 TIME =   44.038
II,JST,KST,LST =  13  1  1  1 NREC =     61 INTLOC =  1667 DEL(TIME) =  19.243 TIME =   63.281
II,JST,KST,LST =  14  1  1  1 NREC =     69 INTLOC =  1262 DEL(TIME) =  22.432 TIME =   85.712
II,JST,KST,LST =  15  1  1  1 NREC =    108 INTLOC =   704 DEL(TIME) =  48.092 TIME =  133.805
II,JST,KST,LST =  16  1  1  1 NREC =    160 INTLOC =  1603 DEL(TIME) =  31.009 TIME =  164.814
II,JST,KST,LST =  17  1  1  1 NREC =    269 INTLOC =  2256 DEL(TIME) =  52.775 TIME =  217.589
II,JST,KST,LST =  18  1  1  1 NREC =    292 INTLOC =   835 DEL(TIME) =  50.056 TIME =  267.644
II,JST,KST,LST =  19  1  1  1 NREC =    398 INTLOC =  1246 DEL(TIME) = 104.842 TIME =  372.486
II,JST,KST,LST =  20  1  1  1 NREC =    530 INTLOC =  1965 DEL(TIME) =  68.116 TIME =  440.602
```
TOTAL NUMBER OF TWO-ELECTRON INTEGRALS =   2137188
THERE IS (ARE)   785 RECORD(S) OF 2E-INTEGRALS WRITTEN ON THE INTEGRAL FILE (IS) (INTLOC = 789)
...... END OF TWO-ELECTRON INTEGRALS ......

The output now displays additional options selected to control the process. Each iteration of the SCF procedure is shown along with the current energy. When the energy no longer can be reduced within the specified tolerance, the calculation is completed and the final energy is listed.

```
********************************

CLOSED-SHELL RHF SCF CALCULATION

********************************

------ NUCLEAR ENERGY ------ =     130.220771462121

              CONVERGENCE DATA
MAXIMUM NUMBER OF ITERATIONS =      40
METHOD OF CONVERGENCE        =      -1
CONVERGENCE CRITERION        =1.0E- 5
PUNCH OUT OPTION             =       2
```

CYCLE		TOTAL ENERGY	ELECTRONIC ENERGY	E CONV.	MAX DIFD	....	DEL(T)	TIME
1	0	-228.420287151	-358.641058614	-358.641058614	0.000000000	....	13.604	586.679
		* * * (RE)INITIATE DIIS PROCEDURE * * *						
2	1	-186.919328524	-317.140099986	41.500958627	17.477428856	....	15.297	601.976
3	2	-244.657119105	-374.877890568	-57.737790581	16.226269580	....	15.302	617.278
4	3	-259.175706643	-389.396478105	-14.518587538	6.444629813	....	15.315	632.592
5	4	-259.549127645	-389.769899107	-0.373421001	0.272430008	....	15.326	647.918
6	5	-259.600026765	-389.820798227	-0.050899120	0.084704848	....	15.338	663.256
7	6	-259.635343256	-389.856114718	-0.035316491	0.059599221	....	15.349	678.605
8	7	-259.638763866	-389.859535328	-0.003420610	0.023140240	....	15.364	693.969
9	8	-259.639342235	-389.860113697	-0.000578369	0.008467660	....	15.374	709.344
10	9	-259.639396828	-389.860168290	-0.000054593	0.002392439	....	15.389	724.732
11	10	-259.639404943	-389.860176405	-0.000008114	0.001083058	....	15.388	740.121
12	11	-259.639405540	-389.860177003	-0.000000598	0.000290452	....	15.387	755.508
13	12	-259.639405650	-389.860177112	-0.000000110	0.000147252	....	15.386	770.894
14	13	-259.639405672	-389.860177134	-0.000000022	0.000055819	....	15.389	786.283
15	14	-259.639405676	-389.860177138	-0.000000004	0.000023296	....	15.389	801.672
16	15	-259.639405676	-389.860177139	-0.000000000	0.000008640	....	15.390	817.062
17	16	-259.639405677	-389.860177139	-0.000000000	0.000002334	....	15.391	832.452

```
DENSITY CONVERGED
```

FINAL ENERGY IS   -259.6394056765 AFTER 17 ITERATIONS

The output then lists the eigenvectors of the molecular orbital.
For the nitramide example this consists of a 64x64 matrix, only a small
portion of which is shown here. The eigenvectors are the coefficients
of each atomic orbital term within the LCAO approximation used to form
the molecular orbitals. The vectors provide an indication of the
contribution of each atomic orbital to each molecular orbital. This
provides a way to understand what each molecular orbital looks like and
what its characteristics are.

EIGENVECTORS

				1	2	3	4	5
				-20.6096	-20.6095	-15.9007	-15.6561	-1.6664
1	1	H	S	-0.000024	0.000015	0.000079	0.000283	-0.018606
2	1	H	S	0.000010	0.000137	-0.000002	0.000447	0.005576
3	2	H	S	0.000028	0.000005	0.000079	0.000284	-0.018600
4	2	H	S	0.000041	0.000131	-0.000002	0.000447	0.005576
5	3	N	S	0.000001	0.000004	-0.001299	0.994922	0.044610

GAMESS then provides a summary of the energy distribution within
the molecule, along with the total energy. Other information that can
be printed out at this point include the Mulliken and Lowdin population
analysis, which show the electron distribution within in the molecular
orbitals; the electron overlap population; the electron gross population
within the atomic orbitals; the electrostatic moments; and the energy
gradient.

ENERGY COMPONENTS

ONE ELECTRON ENERGY =   -613.4231493728
TWO ELECTRON ENERGY =   223.5629722341
NUCLEAR REPULSION ENERGY =   130.2207714621
                                          ─────────────
TOTAL ENERGY =   -259.6394056765

NUCLEUS-ELECTRON POTENTIAL ENERGY =   -872.4594532083
ELECTRON-ELECTRON POTENTIAL ENERGY =   223.5629722341
NUCLEUS-NUCLEUS POTENTIAL ENERGY =   130.2207714621
                                          ─────────────
TOTAL POTENTIAL ENERGY =   -518.6757095120

TOTAL KINETIC ENERGY =   259.0363038355
VIRIAL RATIO (V/T) =   2.0023282522

WAVEFUNCTION NORMALIZATION =   1.0000000000

MULLIKEN AND LOWDIN POPULATION ANALYSES

──────── ALL ELECTRONS ────────

──── TOTAL GROSS POPULATION IN AO'S ────

1	1	H	S	0.49298	0.45288
2	1	H	S	0.10090	0.23583
3	2	H	S	0.49292	0.45043
4	2	H	S	0.10095	0.23580
5	3	N	S	1.99539	1.97732
6	3	N	S	0.77579	0.51725
7	3	N	X	0.77112	0.72384
8	3	N	Y	0.94429	0.90174
9	3	N	Z	0.78414	0.72095
10	3	N	S	0.77639	0.37502
11	3	N	X	0.40096	0.49548
12	3	N	Y	0.65937	0.67016
13	3	N	Z	0.40756	0.46842
14	3	N	XX	0.01380	0.17451
15	3	N	YY	0.00948	0.16531
16	3	N	ZZ	0.03635	0.20077
17	3	N	XY	0.00704	0.01236
18	3	N	XZ	0.01358	0.02294
19	3	N	YZ	0.00644	0.00929
20	4	N	S	1.99572	1.97091
21	4	N	S	0.82813	0.48929
22	4	N	X	0.78253	0.68091
23	4	N	Y	0.67855	0.59909
24	4	N	Z	0.82979	0.72881

25	4	N	S	0.38342	0.25673
26	4	N	X	0.15869	0.33230
27	4	N	Y	0.28816	0.38215
28	4	N	Z	0.07730	0.31149
29	4	N	XX	0.04048	0.19517
30	4	N	YY	0.00113	0.13461
31	4	N	ZZ	0.05309	0.22294
32	4	N	XY	0.02438	0.04876
33	4	N	XZ	0.06889	0.13619
34	4	N	YZ	0.04616	0.09260
35	5	O	S	1.99566	1.97719
36	5	O	S	0.91680	0.72103
37	5	O	X	0.91529	0.86893
38	5	O	Y	0.87069	0.83056
39	5	O	Z	1.04619	1.00495
40	5	O	S	1.00661	0.47701
41	5	O	X	0.49784	0.57359
42	5	O	Y	0.55942	0.61301
43	5	O	Z	0.61462	0.64416
44	5	O	XX	0.01217	0.18377
45	5	O	YY	0.00536	0.17850
46	5	O	ZZ	0.00584	0.17958
47	5	O	XY	0.01108	0.01962
48	5	O	XZ	0.01312	0.02297
49	5	O	YZ	0.00639	0.01125
50	6	O	S	1.99566	1.97727
51	6	O	S	0.91679	0.72366
52	6	O	X	1.12786	1.08692
53	6	O	Y	0.92783	0.88885
54	6	O	Z	0.77650	0.72730
55	6	O	S	1.00660	0.47766
56	6	O	X	0.69622	0.69142
57	6	O	Y	0.62183	0.64538
58	6	O	Z	0.35378	0.48728
59	6	O	XX	0.00230	0.17728
60	6	O	YY	0.00162	0.17729
61	6	O	ZZ	0.02609	0.20166
62	6	O	XY	0.00057	0.00112
63	6	O	XZ	0.00844	0.01587
64	6	O	YZ	0.01494	0.02267

—— CONDENSED TO ATOMS ——

OVERLAP POPULATION (OFF-DIAGONAL ELEMENTS NEED TO BE MULTIPLIED BY 2)

	1	2	3	4	5	6
1	0.3070048					
2	-0.0134869	0.3070137				
3	0.3154793	0.3154670	6.9305454			
4	-0.0283536	-0.0283538	0.2754584	5.3048932		
5	0.0085241	0.0047107	-0.1176258	0.3663769	8.3203004	
6	0.0047114	0.0085225	-0.1176209	0.3664052	-0.1052119	8.3202370

```
          MULLIKEN AND LOWDIN POPULATION
        ATOM        MULL.POP.   CHARGE      LOW.POP.    CHARGE
   1 HYDROGEN       0.593879   0.406121     0.688709   0.311291

   2 HYDROGEN       0.593873   0.406127     0.686226   0.313774

   3 NITROGEN       7.601704  -0.601704     7.435366  -0.435366

   4 NITROGEN       6.256426   0.743574     6.581957   0.418043

   5 OXYGEN         8.477075  -0.477075     8.306105  -0.306105

   6 OXYGEN         8.477043  -0.477043     8.301636  -0.301636
```

ELECTROSTATIC MOMENTS

```
   POINT  1          X          Y         Z (BOHR)    CHARGE
               2.190873   -0.176836    2.979075      0.00 (A.U.)
                   DX         DY         DZ        /D/  (DEBYE)
               -2.717662   2.168777   -2.301926   4.169910
```

If the run type is a geometry optimization or transition state location run, the entire SCF process is repeated at this point. The location of the atoms are altered by the program and a new wavefunction and energy is calculated. The energy is compared to previous runs and continued until an energy minima is reached. The number of iterations can be controlled by the NSERCH parameter so that a search can be limited to conserve computer time if a search gets out of hand. The search data can be written out to a file and restarted.

NSERCH= 21   ENERGY=   -259.6394043

ATOM	ZNUC	COORDINATES (BOHR)			GRADIENT (HARTREE/BOHR)		
		X	Y	Z	X	Y	Z
1 HYDROGEN	1.0	0.5323639	0.4839889	-0.0559817	-0.0001895	-0.0000635	-0.0000732
2 NITROGEN	7.0	0.1836107	0.2929822	1.7868301	0.0001931	-0.0000683	-0.0001604
3 NITROGEN	7.0	2.3504720	-0.~060262	3.0612324	-0.0001322	-0.0001241	0.0003242
4 OXYGEN	8.0	3.9943920	-1.2042457	1.8929916	0.0000822	0.0001404	-0.0000104
5 OXYGEN	8.0	2.3773413	0.3317760	5.2464183	0.0000006	-0.0000516	-0.0001535
6 HYDROGEN	1.0	-0.7681752	1.6900388	2.6207957	0.0000458	0.00C1672	0.0000733

MAXIMUM GRADIENT = 0.0003242   RMS GRADIENT = 0.0001373

When the stationary point is found, the output will say "Equilibrium Geometry Located" and the information that was printed for each search is again printed for the final point. The output printed below shows that it took 21 iterations for the nitramide to reach equilibrium. The eigenvectors are listed now as molecular orbital coefficients, a portion of which is shown below. The charge distribution, electrostatic moment, and overlap are all shown. The program then finishes by closing files and deassigning logical names.

***** EQUILIBRIUM GEOMETRY LOCATED *****

NITRAMIDE 631G* BASIS SET

NUCLEAR COORDINATES (BOHR)

	ATOM	X	Y	Z
1	HYDROGEN	0.532364	0.483989	-0.055982
2	NITROGEN	0.183611	0.292982	1.786830
3	NITROGEN	2.350472	-0.206026	3.061232
4	OXYGEN	3.994392	-1.204246	1.892992
5	OXYGEN	2.377341	0.331776	5.246418
6	HYDROGEN	-0.768175	1.690039	2.620796

INTERNUCLEAR DISTANCES (ANGS.)

		HYDROGEN	NITROGEN	NITROGEN	OXYGEN	OXYGEN	HYDROGEN
1	HYDROGEN	0.0000000	0.9976172	1.9442246	2.2843218	2.9720049	1.6992352
2	NITROGEN	0.9976172	0.0000000	1.3562221	2.1673675	2.1678644	0.9974901
3	NITROGEN	1.9442246	1.3562221	0.0000000	1.1907899	1.1909414	1.9454014
4	OXYGEN	2.2843218	2.1673675	1.1907899	0.0000000	2.1311907	2.9741746
5	OXYGEN	2.9720049	2.1678644	1.1909414	2.1311907	0.0000000	2.2842467
6	HYDROGEN	1.6992352	0.9974901	1.9454014	2.9741746	2.2842467	0.0000000

NUCLEAR ENERGY	=	130.223243931848
ELECTRONIC ENERGY	=	-389.862648202850
TOTAL ENERGY	=	-259.639404271002

MOLECULAR ORBITALS

				1	2	3	4	5	6	7	. . .
				-20.6095	-20.6095	-15.9007	-15.6562	-1.6664	-1.4398	-1.2954	....
1	1	H	S	0.000025	-0.000011	0.000079	-0.000283	-0.018523	0.008255	-0.104270	....
2	1	H	S	0.000008	-0.000137	-0.000003	-0.000447	0.005582	-0.004180	0.009163	....
3	2	N	S	-0.000000	-0.000004	-0.001300	-0.994922	0.044628	0.000018	0.176519	....
4	2	N	S	-0.000004	-0.000072	-0.000129	-0.025129	-0.100210	-0.000024	-0.374941	....
5	2	N	X	0.000022	-0.000054	-0.000188	-0.001094	-0.053252	0.011504	-0.072773	....
6	2	N	Y	-0.000024	0.000002	0.000036	-0.000778	0.005805	-0.010914	-0.033947	....
7	2	N	Z	-0.000053	-0.000023	-0.000107	-0.000180	-0.028395	-0.023838	-0.019933	. ..

—— CONDENSED TO ATOMS ——

OVERLAP POPULATION (OFF-DIAGONAL ELEMENTS NEED TO BE MULTIPLIED BY 2)

	1	2	3	4	5	6
1	0.3070338					
2	0.3154559	6.9304719				
3	-0.0283635	0.2754259	5.3050621			
4	0.0085006	-0.1176510	0.3662526	8.3203854		
5	0.0047064	-0.1175440	0.3665107	-0.1052883	8.3202858	
6	-0.0134671	0.3154702	-0.0283505	0.0047186	0.0085529	0.3069021

MULLIKEN AND LOWDIN POPULATION

ATOM	MULL.POP.	CHARGE	LOW.POP.	CHARGE
1 HYDROGEN	0.593866	0.406134	0.688627	0.311373
2 NITROGEN	7.601629	-0.601629	7.435328	-0.435328
3 NITROGEN	6.256537	0.743463	6.582036	0.417964
4 OXYGEN	8.476918	-0.476918	8.305969	-0.305969
5 OXYGEN	8.477224	-0.477224	8.301864	-0.301864
6 HYDROGEN	0.593826	0.406174	0.686177	0.313823

ELECTROSTATIC MOMENTS

POINT 1	X	Y	Z (BOHR)	CHARGE
	2.211886	-0.170071	2.977940	-0.00 (A.U.)
	DX	DY	DZ	/D/ (DEBYE)
	-2.742149	2.146910	-2.296614	4.171643

STEP CPU TIME = 10.26 TOTAL CPU TIME = 50623.00 (843.7 MIN) IS 84.18 PERCENT OF REAL
TIME OF 60137.09

14840 WORDS OF DYNAMIC MEMORY USED

```
        184320 WORDS OF MEMORY NOT ALLOCATED
EXECUTION OF GAMESS TERMINATED 23-APR-1987 07:59:20
STOP
SJE-I-EXIT,07:59:20, Program exit.
        SHOW/CPU
CPU Usage:              50623.1755 seconds
$ DIRECTORY/SIZE=ALL/DATE SCR:NITR.*


Directory USER$DISK11:[SCRATCH.FPS_SCRATCH]

NITR.DAT;1              3056/3057    23-APR-1987 07:59
NITR.F05;9               2/3         22-APR-1987 14:14
NITR.F05;8               2/3         22-APR-1987 10:26
NITR.F05;7               2/3         26-MAR-1987 14:47
NITR.F10;4             1152/1152     23-APR-1987 08:00
NITR.F10;3             1152/1152     22-APR-1987 12:09
NITR.F10;2              640/642       26-MAR-1987 23:41
NITR.F20;3             3072/3072     23-APR-1987 08:00
NITR.F20;2             3072/3072     22-APR-1987 12:10
NITR.F20;1              128/129       5-MAR-1987 11:00


Total of 10 files, 12278/12285 blocks.
$ COPY SCR:NITR.DAT USER$DISK5:[RODGERSS]NITR.ARC
$ DEL SCR:NITR.DAT;*
$!
$    SHOW TIME
  23-APR-1987 08:01:37
$!
$!   Delete assignments
$!
$ AA:
$    SET NOCONTROL_Y                     ! Continue cleanup if ^Y
$ DEASSIGN IRCDATA
$ DEASSIGN INPUT
$ DEASSIGN OUTPUT
$ DEASSIGN PUNCH
$ DEASSIGN INTGRLS
$ DEASSIGN ORDINT
$ DEASSIGN JKFILE
$ DEASSIGN DICTNRY
$ DEASSIGN DRTFILE
$ DEASSIGN CIVECTR
$ DEASSIGN WORK15
$ DEASSIGN WORK16
$ DEASSIGN DASORT
$    SET CONTROL_Y
$    SET NOVERIFY
  RODGERSS    job terminated at 23-APR-1987 08:01:39.08

  Accounting information:
  Buffered I/O count:        2471    Peak working set size:  1217
  Direct I/O count:        122366    Peak page file size:    2610
  Page faults:               1682    Mounted volumes:           0
  Charged CPU time:   0 00:12:57.63   Elapsed time:    0 17:48:02.07
```

SEMI-EMPIRICAL MOLECULAR ORBITAL (MO) METHOD

The program package MOPAC implements three different methods:
MINDO/3 (modified intermediate neglect of differential overlap) [Ref.
42], MNDO (modified neglect of differential overlap) [Ref. 43], and AM1
(Austin Model 1) [Ref. 44]. The authors of MINDO/3 express the purpose
of these methods best. The purpose "has been to develop a quantum
mechanical treatment of molecular structure and reactivity simple
enough, accurate enough, and reliable enough to serve as a practical
chemical tool in areas at present inaccessible to experimental study.
Typical examples are the properties of transient reaction intermediates,
transition states, and other species involved in the course of chemical
reactions. We envisage the use of computers as the chemical instruments
in a new kind of 'experimental' technique to be used by chemists on the
same kind of basis as infrared or nmr spectroscopy" [Ref. 42].

Background Information

These three methods utilize a frozen core approximation. The core
is composed of the nuclei and inner shell electrons. The valence shell
electrons are then treated using a minimal basis set in which certain
differential overlap terms are neglected. This approach was first put
forth by Pople, et al., and involved the neglect of diatomic
differential overlap (NDDO) [Ref. 45], complete neglect of differential
overlap (CNDO) [Ref. 45], and intermediate neglect of differential
overlap (INDO) [Refs. 46 and 47] approximations.

The CNDO method neglects the electron-repulsion integrals involving
different atomic orbitals centered on the same atom, as well as any

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overlap integrals involving other centers (atoms). This does not lead to a very good representation of a molecular system, but additional parameters used to approximate the frozen core Hamiltonian integrals can be adjusted to give a good overall fit.

The INDO method is an improvement on CNDO since it does not neglect differential overlap between atomic orbitals on the same atom in the one-center electron repulsion integrals. It does, however, still neglect differential overlap in the two-center electron repulsion integrals. Therefore, INDO has more two electron integrals, but is otherwise the same as CNDO [Ref. 48]. The INDO method is the basis for MINDO/3, discussed later in this section.

The last of the three Pople methods is NDDO. This is a further improvement on INDO in which differential overlap is neglected only between AO's centered on different atoms. Since more integrals are included, this method yields better answers. Also, the degree of neglect of differential overlap is much more justifiable in the NDDO approximation [Ref. 48]. NDDO is the basis for MNDO, also discussed later.

Modified INDO (MINDO/3)

MINDO/3 [Ref. 42] is the last improvement of the modified INDO approximation. The terms in the expression for total energy can be placed in five categories: the coulombic interelectronic repulsions, the electron-core attractions, the core-core repulsions, the one-center exchange (resonance) terms, and the two-center exchange terms. In this method, these terms are set to parametric functions which contain numeric parameters which can be modified to agree with experimental

results [Ref. 42].   .

In INDO (and hence MINDO), one must set the repulsion integrals (ii,kk) between AO i of atom m and AO k of atom n to a constant value, γ_{mn}. In this case, the attraction (V_{in}) of an electron in AO i on atom m to the core of atom n can be written as

$$V_{in} = -C_n \gamma_{mn} \tag{12}$$

where C_n is the charge of the atom n core in <u>negative</u> units of electronic charge. These assumptions allow the MINDO Fock matrix to be written as

$$F_{ii} = U_{ii} + \tfrac{1}{2}q_i g_{ii} + \Sigma_{m \neq n}^{(m)}(q_k g_{ik} - \tfrac{1}{2}p_{ik}h_{ik})$$
$$- \Sigma_{n \neq m}\gamma_{mn}(C_n - \Sigma_k^{(n)}g_k) \tag{13}$$

$$F_{ik}(mm) = -\tfrac{1}{2}p_{ik}h_{ik} \tag{14}$$

$$F_{ik}(mn) = \beta_{ik}^c - \tfrac{1}{2}p_{ik}\gamma_{ik} \tag{15}$$

where equation 14 refers to the off-diagonal elements between AO's (i,k) of the same atom (m) and equation 15 refers to those between AO's of different atoms (m and n). $\Sigma^{(p)}$ implies summation over AO's of atom p only, g_{ik} and h_{ik} are the one-center coulomb and exchange integrals between AO's i and k, respectively, β_{ik}^c is the two-center one-electron exchange integral (core resonance integral), U_{ii} is the sum of the kinetic energy of an electron in the AO i of atom m and its potential energy due to attraction by the core of atom m, and q_i and p_{ik} are the

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electron population of AO i and the bond order between AO's i and k, respectively [Ref. 42].

The total energy of a molecule can now be written as

$$E_{tot} = E_{el} + E_c = E_{el} + \Sigma_m \Sigma_n CR_{mn} \qquad (m > n) \qquad (16)$$

where E_{el} is the electronic energy, and E_c is the total core-core repulsion (CR_{mn} is the repulsion between atoms m and n).

From this picture of the total energy, the heat of formation can be obtained. This is done by subtracting the electronic energies E_{el}^A and adding the experimental heats of formation ΔH_f^A of the atoms in the molecule. An assumption here is that the experimental heats of formation for the atoms are the same as the calculated heats of atomization for the atoms.

$$\Delta H_f^{mol} = E_{tot}^{mol} - \Sigma_A E_{el}^A + \Sigma_A \Delta H_f^A \qquad (17)$$

The kinetic energy terms inherent in ΔH_f are taken into account by the parameterization [Refs. 42 and 43].

MINDO/3 parameters must cover three major possible sources of error. These errors are due to the MINDO approximation. The errors are 1) the neglect of coulombic electron correlation, 2) errors introduced in the derivation of the MINDO approximation, and 3) errors from equating calculated energies of atomization to measured heats of atomization [Ref. 42].

To account for the neglect of coulombic electron correlation, one can take advantage of the fact that electron correlation appears to have

no effect on the molecular electron distribution. After calculating

this distribution, the electron repulsion integrals can be reduced to

fit spectroscopic data for the atoms. This accounts for near range

correlation, but long range correlation must be handled in a different

way. Since the only long range electron repulsion integrals are the

γ_{mn}, γ_{mn} must be a function such that as $R_{mn} \rightarrow 0$, the value of the

integral approaches the average of the corresponding one-center

integrals of atoms m and n [Ref. 42].

$$\gamma_{mn} = f_1(R_{mn}) \tag{18}$$

While any well-behaved function satisfying the boundary condition is

suitable, the function selected for MINDO is

$$\gamma_{mn} = e^2[R_{mn}^2 + 0.25(\rho_m + \rho_n)^2]^{-\frac{1}{2}} \tag{19}$$

where

$$\rho_m = e^2/g_m \text{ and } \rho_n = e^2/g_n, \tag{20}$$

g_m and g_n being the one-center integrals on atoms m and n [Ref. 42].

In order to appropriately handle the simplifying assumptions in

MINDO, modifications must be made in the expressions for the core

resonance integrals $\beta_{ik}{}^c$ and the core-core repulsions CR_{mn}. The $\beta_{ik}{}^c$

terms provide the main contribution to molecular bonding energy, and the

equilibrium geometry is determined by balancing the bonding energy

(principally $\beta_{ik}{}^c$) and core-core repulsion (CR_{mn}). If appropriate

functions are chosen for $\beta_{ik}{}^c$ and CR_{mn}, they will be dependent on

molecular geometry. The same functions should be independent of the

atom pairs. However, in order to obtain accurate results, they must contain some parameter for each atom pair [Ref. 42]. This limits MINDO's flexibility.

It has been shown [Ref. 49] that $\beta_{ik}{}^c$ should be proportional to the corresponding overlap integral S_{ik}, and the two corresponding ionization potentials I_i and I_k. This yields the equation

$$\beta_{ik}{}^c = S_{ik}(I_i + I_k)f_2(R_{mn}) \tag{21}$$

where f_2 is a function of R_{mn} and contains an atom pair parameter.

The core-core repulsion is normally equated to the repulsion between two point charges. However, due to the construction of the frozen core approximation, this situation rigidly applies. Therefore, a parametric function must be selected to fit the same boundary conditions as in the two point charge case. The first condition is that the core-core repulsion and the [(core-electron)+(electron-electron)] energies must cancel each other at $R_{mn} = \infty$ for neutral atoms

$$CR_{mn} \rightarrow C_m C_n \gamma_{mn} \quad as \quad R_{mn} \rightarrow \infty. \tag{22}$$

The other condition is that as $R_{mn} \rightarrow 0$, CR_{mn} must become greater than $C_m C_n \gamma_{mn}$. The function for core-core repulsion which will satisfy these boundary conditions is

$$CR_{mn} = C_m C_n [\gamma_{mn} + (e^2 R_{mn}{}^{-1} - \gamma_{mn})f_3(R_{mn})] \tag{23}$$

where f_3 is a function of R_{mn} such that as $R_{mn} \rightarrow \infty$, $f_3 \rightarrow 0$ and as $R_{mn} \rightarrow$

0, $f_3 \to 1$. f_3 also contains the necessary bond pair parameter, as discussed above [Ref. 42].

As can be seen, f_2 and f_3 will be the most empirical functions in this methodology. They are the ones which provide the pathway for closely fitting calculated results to experimental ones. The forms of f_2 and f_3 are found to be

$$f_2 = B_{XY} \quad \text{and} \quad f_3 = \exp(-\alpha_{XY} R_{mn}) \tag{24}$$

where B_{XY} and α_{XY} are the parameters which are characteristic of the atom pair X-Y.

Using this algorithm, parameters were developed which now allow calculations to be performed on the atom pairs shown in Table 6.

Table 6. Allowed MINDO/3 bond pairs [Ref. 50].

	H	B	C	N	O	F	Si	P	S	Cl
H	★	★	★	★	★	★	★	★	★	★
B	★	★	★	★	★	★				
C	★	★	★	★	★	★	★	★	★	★
N	★	★	★	★	★	★			★	★
O	★	★	★	★	★	★			★	★
F	★	★	★	★	★	★			★	
Si	★		★				★			
P	★		★					★		★
S	★		★	★	★	★			★	★
Cl	★		★	★	★			★	★	★

Modified NDDO (MNDO)

The MNDO [Ref. 43] method is based on NDDO. The iterative process of obtaining the total energy is the same as in MINDO/3 (and in MO

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calculations in general), but with the additional two electron repulsion terms present in NDDO (hence MNDO), the Fock matrices are different. In the following equations, the AO's ϕ_μ and ϕ_ν are centered on atom A and AO's ϕ_λ and ϕ_σ are centered on atom B ($A \neq B$). The Fock matrices [Ref. 43] are therefore

$$F_{\mu\mu} = U_{\mu\mu} + \Sigma_B V_{\mu\mu,B} + \Sigma_\nu{}^A P_{\nu\nu}[(\mu\mu,\nu\nu) - \tfrac{1}{2}(\mu\nu,\mu\nu)]$$
$$+ \Sigma_B \Sigma_{\lambda\sigma}{}^B P_{\lambda\sigma}(\mu\mu,\lambda\sigma) \quad (25)$$

$$F_{\mu\nu} = \Sigma_B V_{\mu\nu,B} + \tfrac{1}{2}P_{\mu\nu}[3(\mu\nu,\mu\nu) - (\mu\mu,\nu\nu)] + \Sigma_B \Sigma_{\lambda\sigma}{}^B P_{\lambda\sigma}(\mu\nu,\lambda\sigma) \quad (26)$$

$$F_{\mu\lambda} = \beta_{\mu\lambda} - \tfrac{1}{2}\Sigma_\nu{}^A \Sigma_\sigma{}^B P_{\nu\sigma}(\mu\nu,\lambda\sigma). \quad (27)$$

The total energy and ΔH_f^{mol} are found as in MINDO/3 (equations 16 and 17).

The additional two-electron integrals in the MNDO method allow the modeling of the interactions as multipole-multipole interactions. This approach is different from MINDO/3 and is best explained in the MNDO paper [Ref. 43]. A multipole-multipole interaction function containing a parametric function f_1 is derived. The MNDO f_1 (equation 27) is essentially the same as the MINDO/3 f_1 (equations 18 and 19).

$$f_1(R_{ij}) = [R_{ij}^2 + (\rho^A_{L1} + \rho^B_{L2})^2]^{-\tfrac{1}{2}} \quad (28)$$

Another difference between MNDO and MINDO/3 is in the core-electron attractions (equation 29) and core-core repulsions (equation 30).

$$V_{\mu\nu,B} = -Z_B(\mu^A\mu^A, s^Bs^B) + f_2(R_{AB}) \qquad . \qquad (29)$$

$$E_{AB}{}^{core} = Z_AZ_B(s^As^A, s^Bs^B) + f_3(R_{AB}) \qquad (30)$$

Lastly, as in MINDO/3, an expression for the one-electron resonance integrals, $\beta_{\mu\lambda}$, is derived. It also is assured to be proportional to the corresponding overlap integral $S_{\mu\lambda}$

$$\beta_{\mu\lambda} = f_4(R_{AB})S_{\mu\lambda} \qquad (31)$$

All that remains is to determine the form of the parametric functions f_2-f_4. After extensive testing, the developers decided that f_2 was leading to unrealistic fluctuations in the electronegativities of atoms in a molecule [Ref. 43]. It was therefore set

$$f_2(R_{AB}) = 0. \qquad (32)$$

Given the experience with MINDO, the desire to have more flexibility, and the lack of significant gains by having atom pair parameters, $f_3(R_{AB})$ and $f_4(R_{AB})$ use atomic parameters. The two parametric functions therefore take the form of

$$f_3(R_{AB}) = Z_AZ_B(s^As^A, s^Bs^B)[\exp(-\alpha_AR_{AB}) + \exp(-\alpha_BR_{AB})] \qquad (33)$$

and

$$f_4(R_{AB}) = \tfrac{1}{2}(\beta_\mu{}^A + \beta_\lambda{}^B) \qquad (34)$$

where α and $\beta_\mu{}^A$ are adjustable parameters reflective of the atom and AO

μ on atom A, respectively.

This new algorithm does provide better fit to experiment than MINDO/3 for a variety of different compounds. The elements parameterized for MNDO are H, Li, B, C, N, O, F, Na, Al, Si, P, S, Cl, K, Cr, Ge, Br, Sn, I, Hg, and Pb.

Austin Method 1 (AM1)

The last method in this series is AM1 [Ref. 44]. It is an improvement of MNDO in which a common cause for much of the MNDO error was corrected. This was determined to be that MNDO overestimated the core-core repulsion (CRF) between atoms. This, in general, led to bond lengths longer than experimental values. At first, the search for an improved core repulsion term involved trying to find another function which would be better than the one in MNDO (equations 30 and 33). No other suitable function could be found, so the developers used a "brute force" approach by including more Gaussian terms. The revised core-core repulsion expression used in AM1 is

$$CRF(AB) = Z_A Z_B \gamma_{AB} [1 + F(A) + F(B)] \tag{35}$$

where

$$F(A) = \exp(-\alpha_A R_{AB}) + \Sigma_i K_{Ai} \exp[L_{Ai}(R_{AB} - M_{Ai})^2] \tag{36}$$

$$F(B) = \exp(-\alpha_B R_{AB}) + \Sigma_j K_{Bj} \exp[L_{Bj}(R_{AB} - M_{Bj})^2] \tag{37}$$

The symbolism here is the same as in MNDO. The L parameters determine the width of the Gaussians and since they are not critical, most are set to a common value [Ref. 44].

With this new core repulsion term, the results from AM1 are

improved over the ones from MNDO. The mean absolute errors for heats of formation, dipole moments, and ionization energies are shown in Table III of Ref. 44. Overall, AM1 is the best of the three methods based on having a lower mean absolute error. As the developers state, "we believe that AM1, in its present form, probably represents about the best that can be achieved using the NDDO approximation as a basis, without specific allowance for the contributions of thermal energy" [Ref. 44]. AM1 is parameterized for H, C, N, O, F, Cl, Br, and I.

Installation of MOPAC

The versions received were already prepared to run on the VAX computers. VAX DCL (Digital Control Language) files came with the program to compile and link the code. In addition, DCL files were included to execute the program in batch or interactive mode. These files required modification to site specific directories and batch queues. The modified DCL files are shown in Appendix B.

The advantage in these files is in the ASSIGN statements. Any filename can be given to the input file, and this can be recognized by MOPAC through the logical assignment made by ASSIGN. The DCL files also allow one to select a batch queue other than the default batch queue. The file for doing a batch job is MOPAC.COM. It submits RMOPAC.COM to a batch queue and passes the location of the input file. If one desires to run a job interactively, RMOPAC.COM can be executed. This is not recommended because most jobs will require more than a few minutes.

When compiling MOPAC, a file called DIMSIZES.DAT can be modified to adjust the maximum number of light and heavy (non-hydrogen) atoms. Two considerations are important when deciding the values of these

parameters: what are the largest molecules of interest and what are the system memory settings. The first is self-explanatory. The second is more obtuse. Several system parameters can affect the operation of the program. The most important is the system page file quota. This quota limits the size of a program being loaded and had to be raised to allow a version with 40 heavy and 40 light atoms to be executed.

The MOPAC package was modified so that its progress could be monitored during execution. This was done using the system utility "set process name" (SETPRN). The process name of the job is changed after each cycle to show the cycle just completed and the value of the energy gradient. As the gradient approaches zero, the calculation is nearing completion. This is also useful in determining whether the calculation is oscillating between two local minima with a very small barrier separating them. If this is the case, then the calculation can be terminated.

MOPAC transferred easily over to the FPS attached processor. The only modifications required were the deletion of the VAX-dependent code and different system time-date function calls, both in the subroutine SECOND. The JCL, however, is much different than on the VAX. The program image file and input file have to be copied from the VAX to the FPS, and then the image executed. A serious problem occurred when two different jobs were run back-to-back on the FPS. The first would yield the correct answer, but the second would not. The problem was that some memory registers were not cleared before the second job executed; hence, these values contaminated the results. The solution was to issue a command to clear all registers prior to executing a program.

One other change was made to MOPAC file input/output (I/O). FPS

Fortran provides two options in the OPEN statement for the filename: opening a file on the FPS or opening a file on the host (in this case the VAX). The first option was used initially, and requires that files to be retained must be copied from the FPS to the VAX upon program completion. It was utilized first because I/O from the FPS to the VAX during execution could increase turnaround time on a computation. The second method was tested to provide a comparison to the first. It so happens that most of the I/O occurs at the end of the computation, so there was no noticeable difference in turnaround time. The first method, however, suffers from the fact that with only a scratch disk available, all files are lost if the FPS or host VAX shuts down. The second method avoids this because in the event of a shutdown, all data written up to that point is retained on the VAX. Therefore not all of the work has been lost. This method is the one that has been retained.

Lastly, a version of MOPAC for microcomputers was obtained [Ref. 51]. This version's main limitation is in the amount of memory required. Given the limitation of 640K bytes of memory usable by the MS-DOS operating system, only a 7 heavy and 7 light atom code can be generated. Also, the MS Fortran compiler used to generate the executable code must be version 3.31 or higher. Previous versions of the compiler do not have all the extensions necessary to compile the program. MS-Fortran Version 4.0 was used to compile MOPAC. A test case was run on both the VAX 11/750 and a Zenith Z-248 (8MHz clock speed) microcomputer. The Zenith was found to be approximately 6.5 times slower than the VAX. This performance can be enhanced by linking the program using the 80287 math co-processor library and not the emulator library. However, the Zenith's performance means it can be used to do

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calculations on modest molecular systems.

Outline of MOPAC Work

The plans for MOPAC originally called for an evaluation of its performance on nitro and nitramine containing molecules, to be followed by modification of the parameters, if necessary. Previous work on nitro compounds with MINDO/3 and MNDO indicated these methods did a reasonable job with these compounds, with MINDO/3 giving better heats of formation and MNDO giving better geometries [Ref. 52]. Preliminary testing of AM1 with some of these compounds indicated that problems still existed [Ref. 53]. These considerations led to the aforementioned initial plans for MOPAC. In conversations with one of the developers, however, it was decided that a better course for the semi-empirical work would be to add to the database of calculations on nitro and nitramine containing molecules [Ref. 54]. This database of computations can then be used to modify MOPAC parameters. While work has been done on many nitro containing compounds [Ref. 55], very few nitramines have been done. Therefore, a majority of the compounds calculated in this project were nitramines. The archive files from the computations are included as Appendix A. A discussion of MOPAC's performance on several selected nitramines follows.

Results

The nitramines selected are 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) [Ref. 20], 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) [Ref. 21], N,N-dimethylnitramine (DMN) [Ref. 22], nitramide (nitramine) [Ref. 56], and 7-nitro-5,6-dihydro- 7H-imidazolo[1,2-d]tetrazole (NDIT)

[Ref. 57]. These molecules are displayed in Figures 1-5, respectively.

Calculations on these molecules were done using the three methods and

performed on the VAX 11/750, VAX 11/785, and FPS 164/MAX computers at

the AFAL. Geometry optimizations were performed to determine a stable

conformation. As with most programs, MOPAC is not designed to find the

global minimum and some user interaction is needed. If the input

geometry is very close to a local minimum in the potential energy

hypersurface, it will settle to this local minimum. This is due to the

gradient search routine used to locate a stationary point and follows a

steepest descent logic. Stationary points were found by all methods for

each molecule. The bond length and bond angle data are given in Tables

7-16. The tables display the experimental value, the value calculated

by each method, and the difference between the two (calculated -

experiment) for each bond and bond angle. The numbers associated with

each atom correspond to the atom numbers shown in the figures for each

molecule.

Discussion

Accurate geometries are very important, so a comparison is made

between the calculated geometries and the experimental ones. A point to

remember here is that the calculations are on isolated molecules, so

information from gas phase experiments provide a better measure of

performance. However, x-ray diffraction data was the most commonly

available. The differences between x-ray diffraction and microwave

experiment data are usually limited to bonds involving hydrogen, so use

of x-ray data is justified. Table 17 shows the absolute mean error in

Angstroms for all bond lengths (rows with diatomic representation) and

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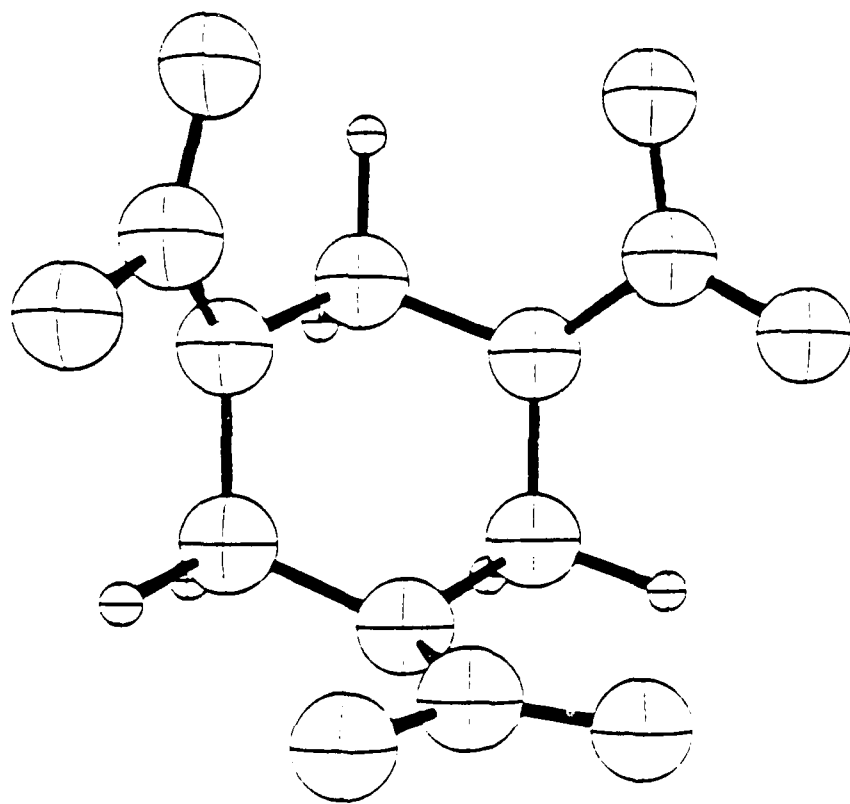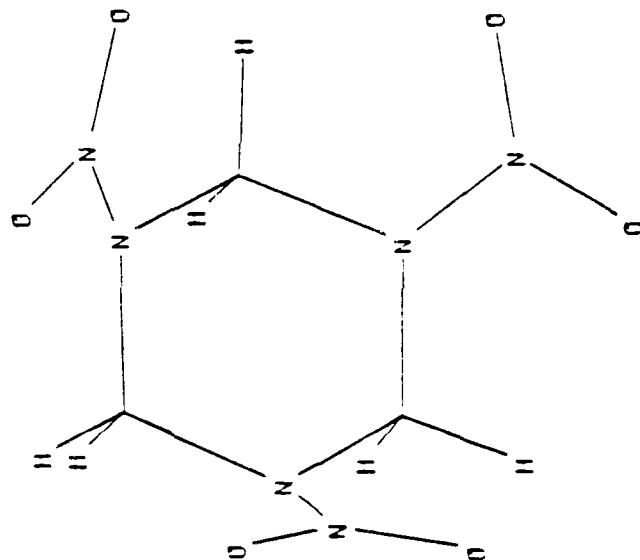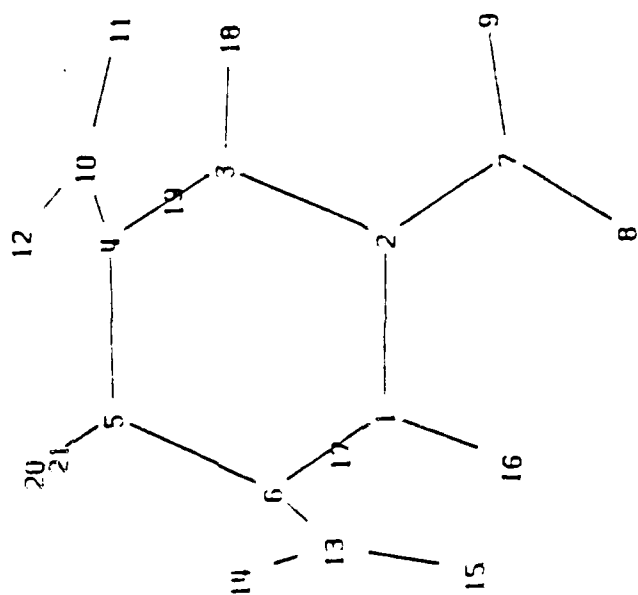
Figure 1. 1,3,5-Trinitro-1,3,5-triazacyclohexane [Ref. 20].

HMX.ANC
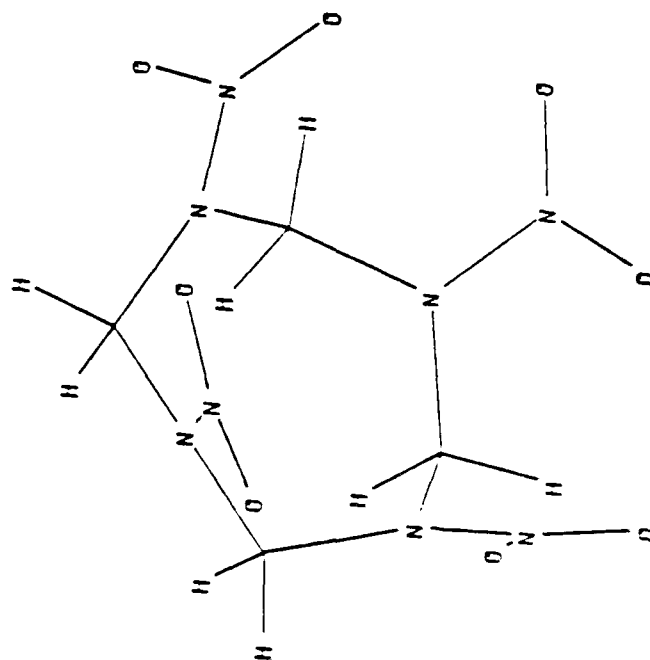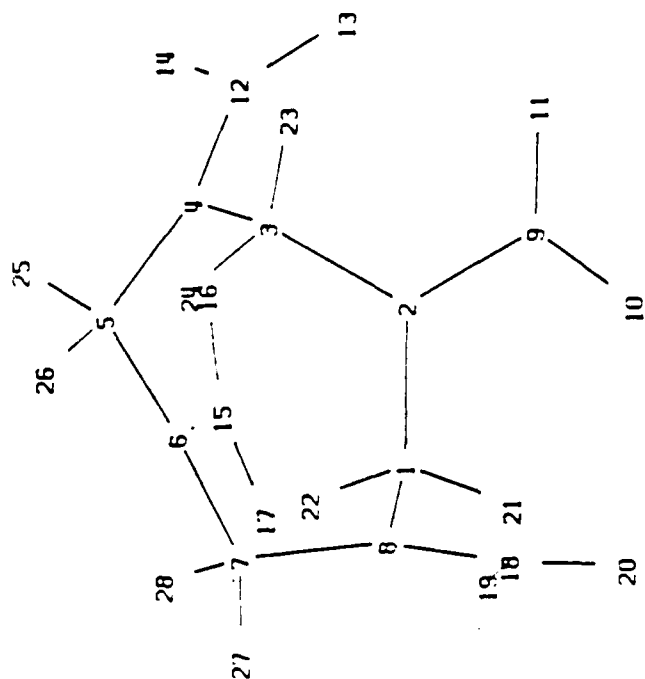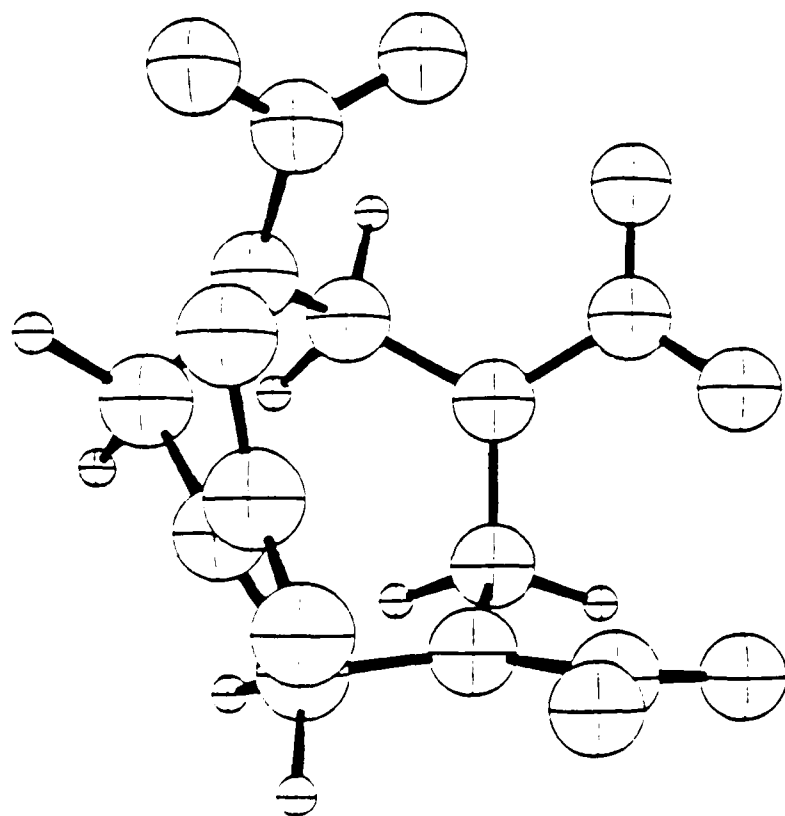
Figure 2. 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane [Ref. 21].

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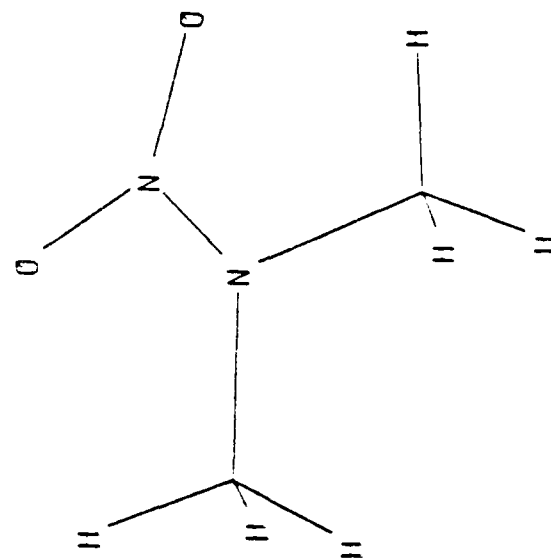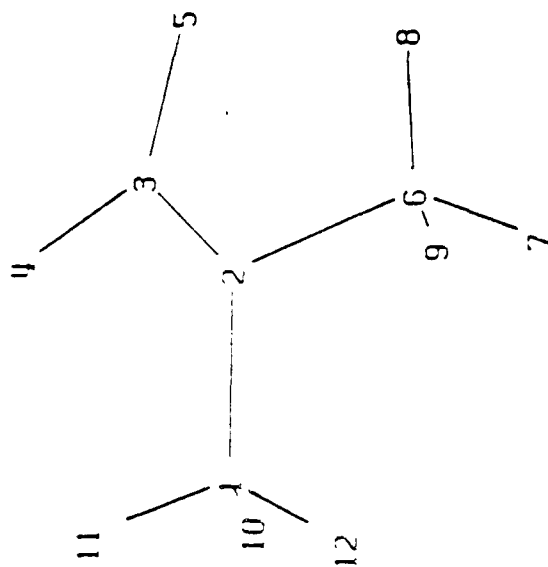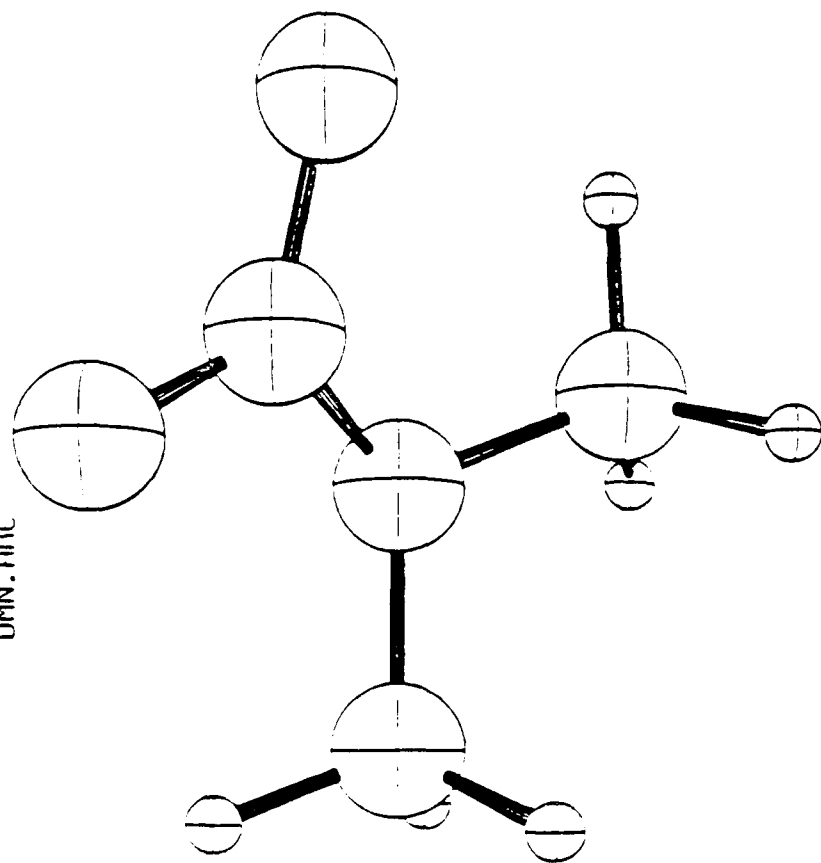
Figure 3. Dimethylnitramide (dimethylnitramine) [Ref. 22].

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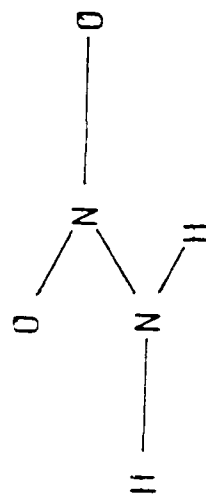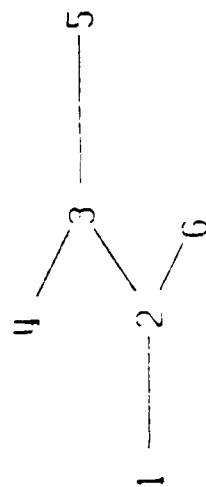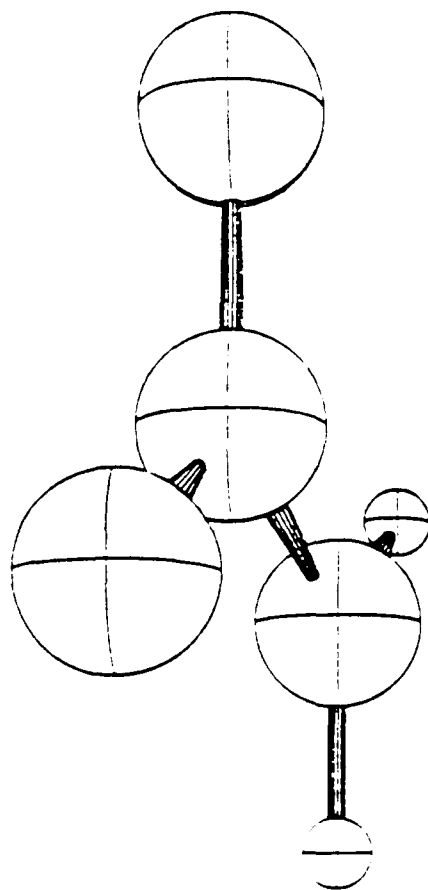
NITRAMIDE.ARC

Figure 4. Nitramide (nitramine) [Ref. 56].

75
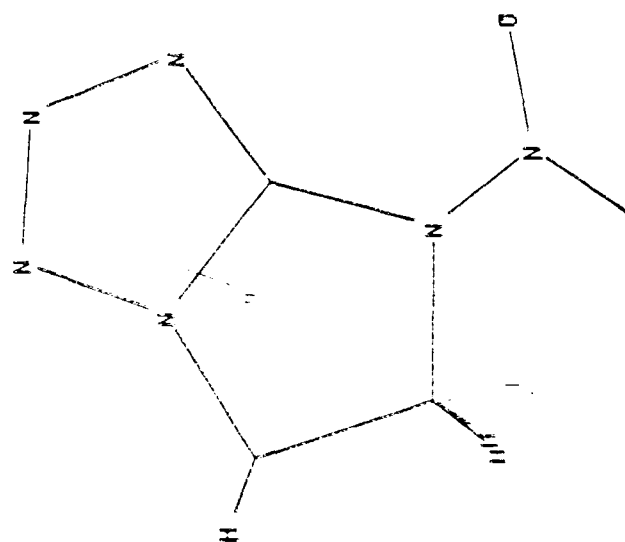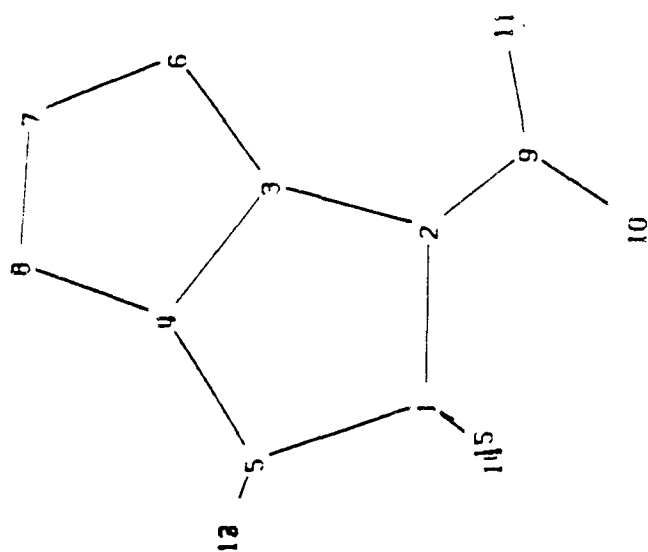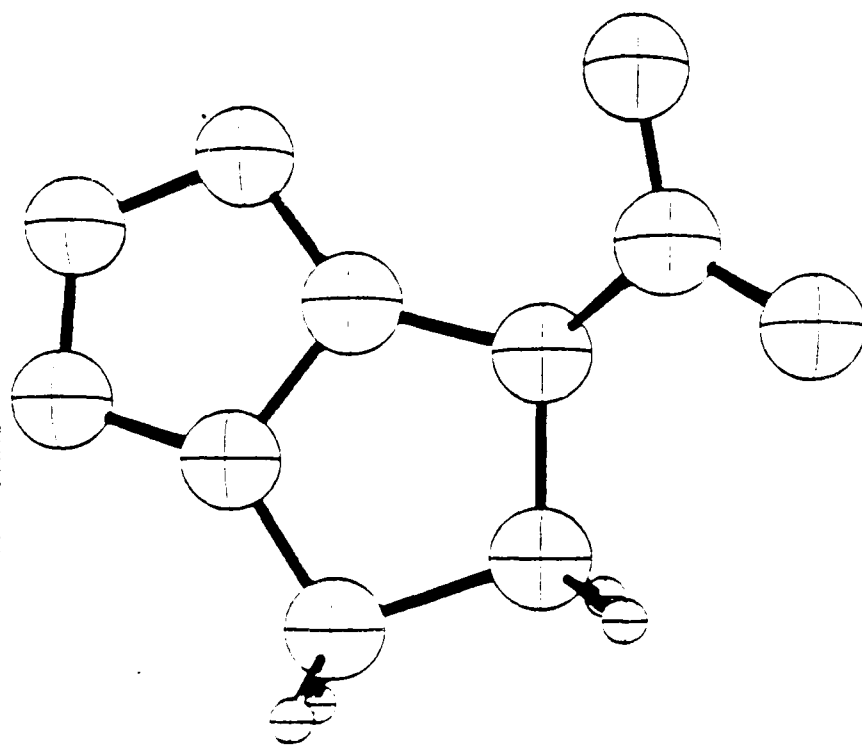
Figure 5. 7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole [Ref. 57].

TABLE 7. Bond lengths of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) (in Angstroms).
Experimental data is from Ref. 20.

BOND	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
C(1)- N(2)	1.4638	1.4576	0.0062	1.4858	0.0220	1.4738	0.0100
C(1)- N(6)	1.4434	1.4553	-0.0119	1.4843	0.0409	1.4746	0.0312
C(1)- H(16)	1.0914	1.1257	-0.0343	1.1166	0.0252	1.1366	0.0452
C(1)- H(17)	1.0592	1.1385	-0.0793	1.1244	0.0652	1.1334	0.0742
N(2)- C(3)	1.4505	1.4555	-0.0050	1.4843	0.0338	1.4743	0.0238
N(2)- N(7)	1.3505	1.3256	0.0249	1.4120	0.0615	1.4171	0.0666
C(3)- N(4)	1.4396	1.4572	-0.0176	1.4857	0.0461	1.4747	0.0351
C(3)- H(18)	1.0749	1.1257	-0.0508	1.1165	0.0416	1.1362	0.0613
C(3)- H(19)	1.0875	1.1386	-0.0511	1.1245	0.0370	1.1334	0.0459
N(4)- C(5)	1.4575	1.4557	0.0018	1.4842	0.0267	1.4741	0.0166
N(4)- N(10)	1.3984	1.3258	0.0726	1.4120	0.0136	1.4169	0.0185
C(5)- N(6)	1.4672	1.4573	0.0099	1.4857	0.0185	1.4739	0.0067
C(5)- H(20)	1.0854	1.1257	-0.0403	1.1166	0.0312	1.1364	0.0510
C(5)- H(21)	1.0871	1.1385	-0.0514	1.1245	0.0374	1.1335	0.0464
N(6)- N(13)	1.3921	1.3258	0.0663	1.4136	0.0215	1.4177	0.0256
N(7)- O(8)	1.2323	1.2261	0.0062	1.2070	-0.0253	1.1987	-0.0336
N(7)- O(9)	1.2093	1.2251	-0.0158	1.2038	-0.0055	1.1987	-0.0106
N(10)- O(11)	1.2046	1.2260	-0.0214	1.2069	0.0023	1.1987	-0.0059
N(10)- O(12)	1.2012	1.2251	-0.0239	1.2039	0.0027	1.1988	-0.0024
N(13)- O(14)	1.2030	1.2260	-0.0230	1.2069	0.0039	1.1987	-0.0043
N(13)- O(15)	1.2068	1.2250	-0.0182	1.2037	-0.0031	1.1988	-0.0080

TABLE 8. Bond angles of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) (in degrees).
Experimental data is from Ref. 20.

ANGLE	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(2)- C(1)- N(6)	107.843	106.082	1.761	110.062	2.219	115.908	8.065
N(2)- C(1)- H(16)	109.982	114.928	-4.946	112.571	2.589	110.493	0.511
N(2)- C(1)- H(17)	109.862	109.639	0.223	106.974	-2.888	105.173	-4.689
N(6)- C(1)- H(16)	110.058	116.001	-5.943	113.128	3.070	110.562	0.504
N(6)- C(1)- H(17)	108.002	110.615	-2.613	107.463	-0.539	105.127	-2.875
H(16)- C(1)- H(17)	111.019	99.429	11.590	106.251	-4.768	109.126	-1.893
C(1)- N(2)- C(3)	115.112	112.030	3.082	115.572	0.460	112.796	-2.316
C(1)- N(2)- N(7)	119.724	123.885	-4.161	119.758	0.034	118.254	-1.470
C(3)- N(2)- N(7)	120.892	124.075	-3.183	118.576	-2.316	118.189	-2.703
N(2)- C(3)- N(4)	108.354	106.184	2.170	109.959	1.605	115.782	7.428
N(2)- C(3)- H(18)	111.470	115.985	-4.515	113.172	1.702	110.526	-0.944
N(2)- C(3)- H(19)	109.636	110.553	-0.917	107.489	-2.147	105.165	-4.471
N(4)- C(3)- H(18)	111.131	114.884	-3.753	112.585	1.454	110.595	-0.536
N(4)- C(3)- H(19)	107.418	109.661	-2.243	107.003	-0.415	105.146	-2.272
H(18)- C(3)- H(19)	108.743	99.414	9.329	106.245	-2.498	109.183	0.440
C(3)- N(4)- C(5)	114.840	112.090	2.750	115.600	0.760	112.613	-2.227
C(3)- N(4)- N(10)	115.607	123.888	-8.281	119.769	4.162	118.261	2.654
C(5)- N(4)- N(10)	117.498	124.017	-6.519	118.609	1.111	118.269	0.771
N(4)- C(5)- N(6)	111.744	106.143	5.601	110.031	-1.713	115.898	4.154
N(4)- C(5)- H(20)	110.709	115.991	-5.282	113.241	2.532	110.522	-0.187

TABLE 8 (continued)

ANGLE	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(4)- C(5)- H(21)	107.191	110.597	-3.406	107.499	0.308	105.118	-2.073
N(6)- C(5)- H(20)	110.095	114.855	-4.760	112.463	2.368	110.605	0.510
N(6)- C(5)- H(21)	106.890	109.655	-2.765	106.959	0.069	105.102	-1.788
H(20)- C(5)- H(21)	110.094	99.449	10.645	106.257	-3.837	109.135	-0.959
C(1)- N(6)- C(5)	114.530	112.100	2.430	115.654	1.124	112.815	-1.715
C(1)- N(6)- N(13)	117.039	124.027	-6.988	118.377	1.338	118.211	1.172
C(5)- N(6)- N(13)	116.652	123.867	-7.215	119.579	2.927	118.184	1.532
N(2)- N(7)- O(8)	117.790	114.337	3.453	118.692	0.902	117.716	-0.074
N(2)- N(7)- O(9)	117.178	114.712	2.466	116.728	-0.450	117.677	0.499
O(8)- N(7)- O(9)	125.010	130.949	-5.939	124.481	-0.529	124.411	-0.599
N(4)- N(10)- O(11)	117.022	114.335	2.687	118.699	1.677	117.701	0.679
N(4)- N(10)- O(12)	117.244	114.688	2.556	116.710	-0.534	117.693	0.449
O(11)- N(10)- O(12)	125.568	130.975	-5.407	124.489	-1.079	124.418	-1.150
N(6)- N(13)- O(14)	117.170	114.320	2.850	118.737	1.567	117.690	0.520
N(6)- N(13)- O(15)	116.811	114.691	2.120	116.639	-0.172	117.714	0.903
O(14)- N(13)- O(15)	125.782	130.987	-5.205	124.530	-1.252	124.404	-1.378

TABLE 9. Bond lengths of 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) (in Angstroms). Experimental data is from Ref. 21.

BOND	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
C(1)- N(2)	1.470	1.4537	-0.0163	1.4785	0.0085	1.4615	-0.0085
C(1)- N(8)	1.451	1.4525	0.0015	1.4761	0.0251	1.4590	0.0080
C(1)- H(21)	1.01	1.1309	0.1209	1.1202	0.1102	1.1384	0.1284
C(1)- H(22)	1.08	1.1376	0.0576	1.1234	0.0534	1.1314	0.0514
N(2)- C(3)	1.472	1.4512	-0.0208	1.4757	0.0037	1.4592	-0.0148
N(2)- N(9)	1.355	1.3447	-0.0103	1.4106	0.0556	1.4094	0.0544
C(3)- N(4)	1.445	1.4555	0.0105	1.4792	0.0342	1.4613	0.0163
C(3)- H(23)	1.01	1.1308	0.1208	1.1201	0.1101	1.1384	0.1284
C(3)- H(24)	1.00	1.1375	0.1375	1.1229	0.1229	1.1314	0.1314
N(4)- C(5)	1.500	1.4528	-0.0472	1.4756	-0.0244	1.4595	-0.0405
N(4)- N(12)	1.363	1.3419	-0.0211	1.4095	0.0465	1.4105	0.0475
C(5)- N(6)	1.475	1.4533	-0.0217	1.4788	0.0038	1.4616	-0.0134
C(5)- H(25)	1.10	1.1310	0.0310	1.1201	0.0201	1.1383	0.0383
C(5)- H(26)	1.00	1.1374	0.1374	1.1229	0.1229	1.1314	0.1314
N(6)- C(7)	1.442	1.4509	0.0089	1.4755	0.0335	1.4590	0.0170
N(6)- N(15)	1.346	1.3447	-0.0013	1.4101	0.0641	1.4083	0.0623
C(7)- N(8)	1.485	1.4552	-0.0298	1.4793	-0.0057	1.4613	-0.0237
C(7)- H(27)	1.03	1.1309	0.1009	1.1202	0.0902	1.1384	0.1084
C(7)- H(28)	1.04	1.1376	0.0976	1.1229	0.0829	1.1315	0.0915
N(8)- N(18)	1.392	1.3418	-0.0502	1.4098	0.0178	1.4105	0.0185
N(9)- O(10)	1.210	1.2221	0.0121	1.2043	-0.0057	1.1990	-0.0110
N(9)- O(11)	1.250	1.2214	-0.0286	1.2052	-0.0448	1.1955	-0.0545
N(12)- O(13)	1.245	1.2229	-0.0221	1.2044	-0.0406	1.1986	-0.0464
N(12)- O(14)	1.212	1.2220	0.0100	1.2051	-0.0069	1.1958	-0.0162
N(15)- O(16)	1.240	1.2220	-0.0180	1.2043	-0.0357	1.1991	-0.0409
N(15)- O(17)	1.187	1.2214	0.0344	1.2050	0.0180	1.1955	-0.0445

TABLE 9 (continued)

BOND	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(18)- O(19)	1.201	1.2229	0.0219	1.2045	0.0035	1.1985	-0.0025
N(18)- O(20)	1.223	1.2219	-0.0011	1.2052	-0.0178	1.1958	-0.0272

TABLE 10. Bond angles of 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) (in degrees). Experimental data is from Ref. 21.

ANGLE	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(2)- C(1)- N(8)	112.8	111.829	-0.971	112.835	0.035	119.054	6.254
N(2)- C(1)- H(21)	109.	111.755	2.755	110.222	1.222	107.705	-1.295
N(2)- C(1)- H(22)	120.	109.190	-10.810	107.885	-12.115	106.198	-13.802
N(8)- C(1)- H(21)	109.	114.560	5.560	111.793	2.793	107.875	-1.125
N(8)- C(1)- H(22)	103.	110.006	7.006	107.979	4.979	106.428	3.428
H(21)- C(1)- H(22)	102.	98.651	-3.349	105.775	3.775	109.320	7.320
C(1)- N(2)- C(3)	121.5	117.580	-3.920	121.485	-0.015	119.534	-1.966
C(1)- N(2)- N(9)	120.8	120.090	-0.710	118.948	-1.852	119.149	-1.651
C(3)- N(2)- N(9)	117.8	121.771	3.971	119.531	1.731	118.865	1.065
N(2)- C(3)- N(4)	112.5	111.531	-0.969	112.513	0.013	118.949	6.449
N(2)- C(3)- H(23)	110.	114.501	4.501	111.896	1.896	107.734	-2.266
N(2)- C(3)- H(24)	108.	110.175	2.175	108.126	0.126	106.578	-1.422
N(4)- C(3)- H(23)	110.	111.976	1.976	110.254	0.254	107.824	-2.176
N(4)- C(3)- H(24)	109.	109.192	0.192	107.887	-1.113	106.150	-2.850
H(23)- C(3)- H(24)	107.	98.667	-8.333	105.837	-1.163	109.357	2.357
C(3)- N(4)- C(5)	116.6	117.092	0.492	121.307	4.707	119.428	2.828
C(3)- N(4)- N(12)	119.4	120.307	0.907	119.041	-0.359	119.156	-0.244
C(5)- N(4)- N(12)	118.7	122.024	3.324	119.611	0.911	118.774	0.074
N(4)- C(5)- N(6)	108.5	111.690	3.190	112.369	3.869	118.693	10.193
N(4)- C(5)- H(25)	111.	114.489	3.489	111.985	0.985	107.923	-3.077
N(4)- C(5)- H(26)	100.	110.070	10.070	108.144	8.144	106.515	6.515
N(6)- C(5)- H(25)	108.	111.767	3.767	110.247	2.247	107.862	-0.138
N(6)- C(5)- H(26)	91.	109.300	18.300	107.952	16.952	106.266	15.266
H(25)- C(5)- H(26)	135.	98.716	-36.284	105.824	-29.176	109.339	-25.661
C(5)- N(6)- C(7)	119.3	117.445	-1.855	121.317	2.017	119.495	0.195
C(5)- N(6)- N(15)	117.2	120.215	3.015	119.027	1.827	119.230	2.030
C(7)- N(6)- N(15)	123.5	121.806	-1.694	119.617	3.883	119.036	-4.464
N(6)- C(7)- N(8)	113.0	111.698	-1.302	112.773	-0.227	118.919	5.919
N(6)- C(7)- H(27)	92.	114.470	22.470	111.877	19.877	107.739	15.739
N(6)- C(7)- H(28)	108.	110.095	2.095	108.131	0.131	106.596	-1.404
N(8)- C(7)- H(27)	107.	111.900	4.900	110.138	3.138	107.801	0.801
N(8)- C(7)- H(28)	109.	109.194	0.194	107.760	-1.240	106.166	-2.834
H(27)- C(7)- H(28)	128.	98.660	-29.340	105.814	-22.186	109.377	-18.623
C(1)- N(8)- C(7)	119.6	117.123	-2.477	121.374	1.774	119.222	-0.378
C(1)- N(8)- N(18)	120.8	121.979	1.179	119.420	-1.380	118.892	-1.908
C(7)- N(8)- N(18)	118.6	120.345	1.745	119.093	0.493	119.210	0.610
N(2)- N(9)- O(10)	119.9	113.482	-6.418	117.952	-1.948	117.460	-2.440
N(2)- N(9)- O(11)	114.2	114.775	0.575	117.385	3.185	117.375	3.175
O(10)- N(9)- O(11)	126.0	131.715	5.715	124.615	-1.385	125.074	-0.926
N(4)- N(12)- O(13)	117.7	113.518	-4.182	117.987	0.287	117.502	-0.198

TABLE 10 (continued)

ANGLE	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(4)- N(12)- O(14)	120.3	114.920	-5.380	117.420	-2.880	117.329	-2.971
O(13)- N(12)- O(14)	121.3	131.532	10.232	124.541	3.241	125.067	3.767
N(6)- N(15)- C(16)	115.1	113.511	-1.589	117.968	2.868	117.400	2.300
N(6)- N(15)- O(17)	122.1	114.727	-7.373	117.384	-4.716	117.435	-4.665
O(16)- N(15)- O(17)	122.7	131.734	9.034	124.595	1.895	125.080	2.380
N(8)- N(18)- O(19)	116.6	113.526	-3.074	118.078	1.478	117.498	0.898
N(8)- N(18)- O(20)	116.2	114.919	-1.281	117.350	1.150	117.272	1.072
O(19)- N(18)- O(20)	127.3	131.525	4.225	124.512	-2.788	125.125	-2.175

TABLE 11. Bond lengths of dimethylnitramide (DMN) (in Angstroms). Experimental data is from Ref. 22.

BOND	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
C(1)- N(2)	1.461	1.4463	-0.015	1.4860	0.025	1.4578	-0.003
C(1)- H(10)	1.090	1.1187	0.029	1.1140	0.024	1.1218	0.032
C(1)- H(11)	1.110	1.1180	0.008	1.1119	0.002	1.1228	0.013
C(1)- H(12)	1.060	1.1182	0.058	1.1128	0.053	1.1226	0.063
N(2)- N(3)	1.323	1.3110	-0.012	1.3951	0.072	1.4099	0.087
N(2)- C(6)	1.457	1.4463	-0.011	1.4858	0.029	1.4578	0.001
N(3)- O(4)	1.233	1.2315	-0.002	1.2106	-0.022	1.2029	-0.030
N(3)- O(5)	1.244	1.2315	-0.012	1.2106	-0.033	1.2030	-0.041
C(6)- H(7)	1.080	1.1189	0.039	1.1118	0.032	1.1226	0.043
C(6)- H(8)	1.040	1.1178	0.078	1.1141	0.074	1.1228	0.083
C(6)- H(9)	1.110	1.1183	0.008	1.1129	0.003	1.1218	0.012

TABLE 12. Bond angles of dimethylnitramide (DMN) (in degrees). Experimental data is from Ref. 22.

ANGLE	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(2)- C(1)- H(10)	106.7	114.415	7.715	112.445	5.745	106.300	-0.400
N(2)- C(1)- H(11)	110.6	114.896	4.296	111.089	0.489	110.773	0.173
N(2)- C(1)- H(12)	110.3	111.842	1.542	108.512	-1.788	112.172	1.872
H(10)- C(1)- H(11)	111.0	106.521	-4.479	109.195	-1.805	108.944	-2.056
H(10)- C(1)- H(12)	109.6	104.232	-5.368	108.282	-1.318	109.487	-0.113
H(11)- C(1)- H(12)	109.0	103.864	-5.136	107.135	-1.865	109.086	0.086
C(1)- N(2)- N(3)	117.2	122.068	4.868	117.930	0.730	116.914	-0.286
C(1)- N(2)- C(6)	124.2	115.839	-8.361	116.726	-7.474	113.211	-10.989
N(3)- N(2)- C(6)	117.5	122.091	4.591	118.025	0.525	116.838	-0.662
N(2)- N(_3)- O(4)	118.3	114.930	-3.370	118.608	0.308	118.293	-0.007
N(2)- N(3)- O(5)	118.4	114.909	-3.491	118.654	0.254	118.303	-0.097
O(4)- N(3)- O(5)	123.3	130.160	6.860	122.602	-0.698	123.195	-0.105
N(2)- C(6)- H(7)	108.3	114.288	5.988	111.203	2.903	112.254	3.954
N(2)- C(6)- H(8)	112.4	114.987	2.587	112.431	0.031	110.611	-1.789

TABLE 12 (continued)

ANGLE	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(2)– C(6)– H(9)	108.1	111.834	3.734	108.417	0.317	106.316	-1.784
H(7)– C(6)– H(8)	103.9	106.514	2.614	109.195	5.295	109.116	5.216
H(7)– C(6)– H(9)	115.7	104.357	-11.343	107.100	-8.600	109.508	-6.192
H(8)– C(6)– H(9)	108.5	103.800	-4.700	108.308	-0.192	108.957	0.457

TABLE 13. Bond lengths of nitramide (in Angstroms). Experimental data is from Ref. 56.

BOND	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
O(1)– N(2)	1.206	1.2295	0.024	1.2090	0.003	1.2044	-0.002
N(2)– N(3)	1.427	1.2870	-0.140	1.4064	-0.021	1.3674	-0.060
N(·– O(6)	1.206	1.2295	0.024	1.2091	0.003	1.2044	-0.002
N(3)– H(4)	1.005	1.0273	0.022	1.0178	0.013	1.0023	-0.003
N(3)– H(5)	1.005	1.0273	0.022	1.0178	0.013	1.0023	-0.003

TABLE 14. Bond angles of nitramide (in degrees). Experimental data is from Ref. 56.

ANGLE	EXP[a]	MINDO/3	Δ	MNDO	Δ	AM1	Δ
O(1)– N(2)– N(3)	114.93	113.917	-1.013	117.817	2.887	117.971	3.041
O(1)– N(2)– O(6)	130.25	132.172	1.922	124.129	-6.121	123.988	-6.262
N(3)– N(2)– O(6)	114.93	113.911	-1.019	117.808	2.878	117.964	3.034
N(2)– N(3)– H(4)	122.41	125.857	3.447	112.237	-10.173	114.204	-8.206
N(2)– N(3)– H(5)	122.41	125.841	3.431	112.221	-10.189	114.203	-8.207
H(4)– N(3)– H(5)	115.18	108.302	-6.878	107.451	-7.729	117.408	2.228

[a]The only angles reported in the reference were the O–N–O and H–N–H angles. The others were determined by subtracting the value of the reported angle from 360 and dividing the remainder by 2. This gave values for N–N–O angles (from O–N–O) and for N–N–H angles (from H–N–H).

TABLE 15. Bond lengths of 7-nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole (NDIT) (in Angstroms). Experimental data is from Ref. 57.

BOND	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
C(1)– N(2)	1.4898	1.4771	-0.0127	1.5151	0.0253	1.5020	0.0122
C(1)– C(5)	1.5414	1.5215	-0.0199	1.5693	0.0279	1.5732	0.0318
C(1)– H(14)	0.9561	1.1251	0.1690	1.1142	0.1581	1.1229	0.1668
C(1)– H(15)	0.9566	1.1251	0.1685	1.1136	0.1570	1.1228	0.1662

TABLE 15 (continued)

BOND	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(2)- C(3)	1.3656	1.4051	0.0395	1.4106	0.0450	1.4292	0.0636
N(2)- N(9)	1.3563	1.3050	-0.0513	1.4153	0.0590	1.4363	0.0800
C(3)- N(4)	1.3221	1.3917	0.0696	1.4041	0.0820	1.4417	0.1196
C(3)- N(6)	1.3049	1.3284	0.0235	1.3471	0.0422	1.3646	0.0597
N(4)- C(5)	1.4311	1.4410	0.0099	1.4670	0.0359	1.4509	0.0198
N(4)- N(8)	1.3549	1.2999	-0.0550	1.3402	-0.0147	1.3333	-0.0216
C(5)- H(12)	0.9664	1.1252	0.1588	1.1133	0.1469	1.1222	0.1558
C(5)- H(13)	0.9665	1.1252	0.1587	1.1134	0.1469	1.1221	0.1556
N(6)- N(7)	1.3657	1.2880	-0.0777	1.3365	-0.0292	1.3408	-0.0249
N(7)- N(8)	1.3129	1.2248	-0.0881	1.2769	-0.0360	1.2883	-0.0246
N(9)- O(10)	1.1936	1.2305	0.0369	1.2027	0.0091	1.2001	0.0065
N(9)- O(11)	1.2228	1.2304	0.0076	1.2063	-0.0165	1.1924	-0.0304

TABLE 16. Bond angles of 7-nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole (NDIT) (in degrees). Experimental data is from Ref. 57.

ANGLE	EXP	MINDO/3	Δ	MNDO	Δ	AM1	Δ
N(2)- C(1)- C(5)	101.740	106.379	4.639	107.329	5.589	108.906	7.166
N(2)- C(1)- H(14)	108.378	112.622	4.244	107.494	-0.884	112.554	4.176
N(2)- C(1)- H(15)	111.073	112.609	1.536	112.562	˙1.489	105.254	-5.819
C(5)- C(1)- H(14)	109.981	111.409	1.428	111.177	1.196	110.368	0.387
C(5)- C(1)- H(15)	115.847	111.414	-4.433	110.191	-5.656	110.303	-5.544
H(14)- C(1)- H(15)	109.422	102.538	-6.884	108.087	-1.335	109.340	-0.082
C(1)- N(2)- C(3)	111.825	108.544	-3.281	106.949	-4.876	104.678	-7.147
C(1)- N(2)- N(9)	123.190	127.261	4.071	120.185	-3.005	117.634	-5.556
C(3)- N(2)- N(9)	124.420	124.195	-0.225	120.255	-4.165	116.867	-7.553
N(2)- C(3)- N(4)	107.679	108.935	1.256	110.536	2.857	112.723	5.044
N(2)- C(3)- N(6)	141.012	145.418	4.406	142.174	1.162	141.058	0.046
N(4)- C(3)- N(6)	111.309	105.647	-5.662	106.896	-4.413	106.034	-5.275
C(3)- N(4)- C(5)	115.429	112.578	-2.851	113.535	-1.894	110.476	-4.953
C(3)- N(4)- N(8)	108.624	107.741	-0.883	107.387	-1.237	107.566	-1.058
C(5)- N(4)- N(8)	135.944	139.681	3.737	138.418	2.474	140.975	5.031
C(1)- C(5)- N(4)	102.971	103.563	0.592	101.364	-1.607	103.160	0.189
C(1)- C(5)- H(12)	111.336	111.858	0.522	112.547	1.211	110.618	-0.718
C(1)- C(5)- H(13)	109.265	111.841	2.576	112.122	2.857	111.624	2.359
N(4)- C(5)- H(12)	106.041	114.183	8.142	111.048	5.007	111.347	5.306
N(4)- C(5)- H(13)	113.683	114.160	0.477	111.720	-1.963	110.218	-3.465
H(12)- C(5)- H(13)	113.091	101.581	-11.510	108.016	-5.075	109.743	-3.348
C(3)- N(6)- N(7)	103.333	103.714	0.381	104.804	1.471	104.493	1.160
N(6)- N(7)- N(8)	112.716	117.327	4.611	114.364	1.648	115.365	2.649
N(4)- N(8)- N(7)	104.009	105.571	1.562	106.509	2.500	106.469	2.460
N(2)- N(9)- O(10)	116.028	113.829	-2.199	118.881	2.853	116.465	0.437
N(2)- N(9)- O(11)	115.293	115.141	-0.152	116.069	0.776	118.397	3.104
O(10)- N(9)- O(11)	128.679	131.030	2.351	124.883	-3.796	124.896	-3.783

TABLE 17. Absolute mean errors for bond lengths (diatomic representation, Angstroms) and bond angles (triatomic representation, degrees)[a].

	HMX			RDX			NDIT		
	MINDO/3	MNDO	AM1	MINDO/3	MNDO	AM1	MINDO/3	MNDO	AM1
C-N	0.02(-)	0.02(+)	0.02(-)	0.01(0)	0.03(+)	0.02(+)	0.03(+)	0.05(+)	0.06(+)
C-H	0.10(+)	0.09(+)	0.10(+)	0.05(+)	0.04(+)	0.05(+)	0.16(+)	0.15(+)	0.16(+)
N-O	0.02(0)	0.02(-)	0.03(-)	0.02(+)	0.01(0)	0.01(-)	0.02(+)	0.04(+)	0.02(0)
N-N	0.02(-)	0.05(+)	0.05(+)	0.06(-)	0.03(+)	0.04(+)	0.07(-)	0.01(0)	0.04(-)
C-C							0.02(-)	0.03(+)	0.03(+)
N-H									
N-C-N	1.61(-)	1.04(+)	7.20(+)	3.18(-)	1.84(+)	6.55(+)	3.77(+)	2.81(+)	3.46(+)
N-C-H	6.27(+)	4.83(+)	4.63(-)	3.45(+)	1.67(+)	1.43(-)	3.60(+)	2.34(0)	4.69(0)
C-N-C	2.19(-)	2.13(+)	1.34(0)	2.75(-)	0.78(+)	2.09(-)	3.07(-)	3.38(-)	6.05(-)
N-N-O	3.73(-)	2.31(+)	2.21(0)	2.69(-)	0.88(0)	0.52(+)	1.18(-)	1.81(+)	1.77(+)
O-N-O	7.30(+)	2.33(0)	2.31(0)	5.52(+)	0.95(-)	1.04(-)	2.35(+)	3.80(-)	3.78(-)
N-N-C	2.07(+)	1.55(+)	1.51(0)	6.06(+)	1.98(+)	1.72(+)	1.86(+)	2.47(-)	4.07(-)
H-C-H	19.33(-)	14.08(-)	13.49(0)	10.52(-)	3.70(-)	1.10(-)	9.20(-)	3.20(-)	1.72(-)
N-C-C							2.62(+)	3.60(0)	3.68(+)
C-C-H							2.24(+)	2.73(+)	2.25(0)
N-N-N							3.09(+)	2.07(+)	2.55(+)
N-N-H									
H-N-H									

	DMN			NITRAMIDE		
	MINDO/3	MNDO	AM1	MINDO/3	MNDO	AM1
C-N	0.01(-)	0.03(+)	0.00(0)			
C-H	0.04(+)	0.03(+)	0.04(+)			
N-O	0.01(-)	0.03(-)	0.04(-)	0.02(+)	0.00(+)	0.00(-)
N-N	0.01(-)	0.07(+)	0.09(+)	0.14(-)	0.02(-)	0.06(-)
C-C						
N-H				0.02(+)	0.01(+)	0.00(-)
N-C-N						
N-C-H	4.31(+)	1.88(+)	1.66(0)			
C-N-C	8.36(-)	7.47(-)	10.99(-)			
N-N-O	3.43(-)	0.28(+)	0.05(-)	1.02(-)	2.88(+)	3.04(+)
O-N-O	6.86(+)	0.70(-)	0.10(-)	1.92(+)	6.12(-)	6.26(-)
N-N-C	4.73(+)	0.63(+)	0.47(-)			
H-C-H	5.61(-)	3.18(-)	2.35(0)			
N-C-C						
C-C-H						
N-N-N						
N-N-H				3.44(+)	10.18(-)	8.21(-)
H-N-H				6.88(-)	7.73(-)	2.23(+)

[a]The +, -, and 0 are the trend in the method's estimate. It was determined by counting the number of parameters overestimated (+) and underestimated (-). If there were more overestimated, a (+) is shown; if more underestimated, a (-); and if an equal number of each, then (0).

in degrees for bond angles (rows with triatomic representation), along with the trend (+, -, or 0) in the error. The + means the method overestimated a particular parameter more times than the method underestimated, - means just the opposite, and 0 means there was an equal number of parameters under- and over-estimated. There are some similarities and differences between these five molecules. RDX and HMX are both cyclic nitramines; NDIT is bicyclic but with an -N-N-N- ring moiety; DMN is the simplest disubstituted nitramine (R_2NNO_2); nitramide is the parent (and simplest) nitramine. The atoms and large subgroups ($-CH_2-$, $>NNO_2$, etc...) are in different molecular environments and will influence the calculations.

Bond Lengths

With this in mind, one can now examine the consistency of each method for the parameters in each molecule. In general, C-H bond lengths tend to be overestimated. This is because the listed experimental data is from x-ray or neutron diffraction experiments, except nitramide, which is from a microwave experiment. An x-ray experiment determines atom positions by the scattering of the x-rays off the atoms, or more precisely, the electron density. In C-H bonds, electron density is shifted from the hydrogen towards the carbon and so the bond seems "shorter." This is the case for HMX and NDIT. The structure of RDX was determined by neutron diffraction, where nuclei scatter the neutrons. This kind of experiment gives better positions for hydrogens. The DMN data is from a low temperature (85K) x-ray experiment where thermal uncertainties are reduced and the hydrogen positions more accurately determined.

The N-N bond lengths with MINDO/3 tend to be underestimated by a large amount, but appear to be influenced strongly by the strain present in the molecule. This is why RDX and NDIT have large errors, while HMX and DMN do not. MNDO, and especially AM1, have a generally larger error with no discernible trend. The differences between these two methods and MINDO/3 may lie in the nature of their basic approximations (NDDO vs INDO) and parameters (atomic vs bond pair). Another possibility is the neglect of the cyclic nitramine strain energy in the parameterization process. Nitramide appears to behave differently than any of the other nitramines. The differences are most likely due to the presence of hydrogens on the amine nitrogen rather than carbons. The N-N bond length is much longer than in other nitramines, and MNDO does very well on reproducing this fact. MINDO/3, on the other hand, does a very poor job on the N-N bond length. The N-H bond length is handled well by all methods, but this is because the experimental data is from a microwave experiment, not an x-ray diffraction experiment. Studies on other central N-N bond systems (N_2H_4, N_2O_4, F_2NNO_2, H_2NNF_2) may prove interesting. Some of these compounds are good fuels and oxidizers and this fact is probably strongly dependent on the nature of the N-N bond. The C-N bond seems to be handled well by all the methods. The exception in NDIT is most likely due to the bicyclic ring strain.

Bond Angles

The bond angles are more consistent among the molecules. With few exceptions, both AM1 and MNDO do a good job in reproducing the experimental data. AM1 appears to have some difficulty handling the N-C-N angles, always tending to overestimate. It also seems to have

some problems with the C-N-C angles, but only in NDIT and DMN. All

three methods had problems with the H-C-H angles in HMX and with the

C-N-C angles in DMN. This implies that the molecular environments in

these two systems have a dramatic effect on the calculations. These

exceptions were the only ones where AM1 and MNDO failed to reproduce the

bond angles to within 5°. MINDO/3, on the other hand, gave

significantly larger errors for all angles than the other two methods.

This is in agreement with earlier work [Ref. 52].

Heats of Formation (ΔH_f)

The calculated heats of formation (ΔH_f) for these five molecules

are shown in Table 18.

Table 18. Heats of formation (ΔH_f) for selected nitramines (25°C) in kcal/mole.

	Exp	MINDO/3	Δ	MNDO	Δ	AM1	Δ
RDX	14.7[a,b]	-34.5	-49.2	102.9	88.2	105.1	90.4
HMX	17.9[a,b]	-29.1	-47.0	149.2	131.3	144.4	136.5
DMN	-3.2[b,c]	-9.6	-7.4	22.9	26.1	21.7	24.9
Nitramide	--	-29.8	--	19.4	--	12.9	--
NDIT	--	-58.5	--	99.2	--	177.0	--

[a]See reference 24. [b]See reference 25. [c]See reference 26.

Experimental values for many nitramines are not available, but are found

for RDX, HMX, and DMN. One can see that the methods do not reproduce

heat of formation data very well at all. This kind of error limits the

usefulness of the methods for propulsion applications because a very

accurate ΔH_f is required to predict propellant performance. However,

activation energies for chemical reactions might be accurate enough

using the methods. This is based on the supposition that the relative energy between two systems will be accurately reproduced (e.g., any error in the reactants and products is the same). This would almost certainly be true in isodesmic systems, but not necessarily so in other systems. The source of the error may find its root in one of three places: the total energy of the system, the electronic energy of the system, or the assumption equating calculated heats of atomization with experimental heats of atomization (see equation 17). In either of the first two cases, modifications to the parametric functions or to the parameters may be necessary to overcome the ΔH_f deficiency.

Summary

In general, MNDO and AM1 provide better geometries than MINDO/3. The errors indicate that overall MNDO and AM1 yield geometries very close to each other. These geometries are close to experimental ones since the error is confined, in general, to less than 0.05Å for bond angles. In order to reflect the subtle differences due to molecular environment, however, it is desirable to improve the error in the bond lengths to be less than 0.02Å. The bond angles are accurate enough to provide good interpretation of calculated properties.

With the heats of formation, much work is needed to improve all the methods' performance. This can only be accomplished by having a large database of computations with which to compare to experiment. After a database has been established, it will be possible to methodically alter parameters to improve accuracy. It is desirable to get ΔH_f within about 5 kcal/mole of the experimental value for use with estimation of propellant performance.

CONCLUSIONS

The Prediction of Molecular Properties project has brought a powerful set of tools to the AFAL. The computational chemistry programs installed can be used in basic chemical research to attack different problems. MM2 can be used to quickly determine molecular geometries. MOPAC can be used to follow reaction pathways and predict other properties such as heat of formation, ionization energy, dipole moment, and infrared spectra. The ab initio programs can be used to provide accurate, detailed descriptions of molecular geometries and properties.

There are a large number of potential applications for these methods at the AFAL. Similar to setting up a laboratory experiment (such as a synthesis procedure), it is possible to design a computer "experiment" to determine answers to various chemical questions. Some areas where computations can be used are in designing a molecular synthesis route, examining combustion reaction chemistry, looking at polymer reactivity and mechanical properties, potential interactions of solar radiation with molecular systems, the gas phase chemistry occurring in exhaust plumes, infrared signatures, and modeling of molecular clusters as a means of storing otherwise transient species (metastable molecules and antimatter).

The capability established at the AFAL is a basic one. It allows researchers to perform good, publishable calculations on a wide variety of molecular systems. However, programs are available which are designed to address specific chemical problems (macromolecules, clusters, solution chemistry, to name a few). These can provide insight into the chemical problems affecting propulsion system performance. It

is hoped that this project will provide AFAL researchers with a valuable tool for tackling propulsion problems.

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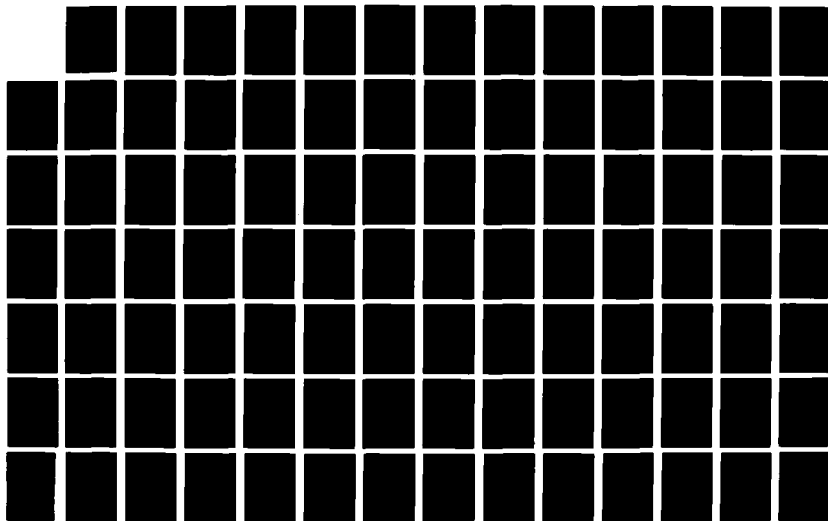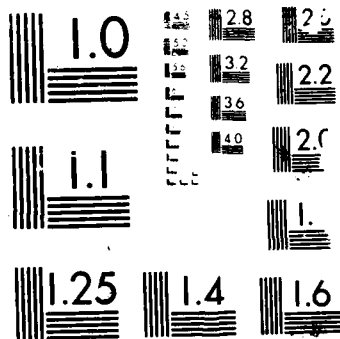
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APPENDIX A

TABLE OF CONTENTS/LIST OF FIGURES*

*All molecular drawings were done using the program DRAW, written by Major Donn Storch, Department of Chemistry, USAF Academy, CO.

ANANPZ.ARC
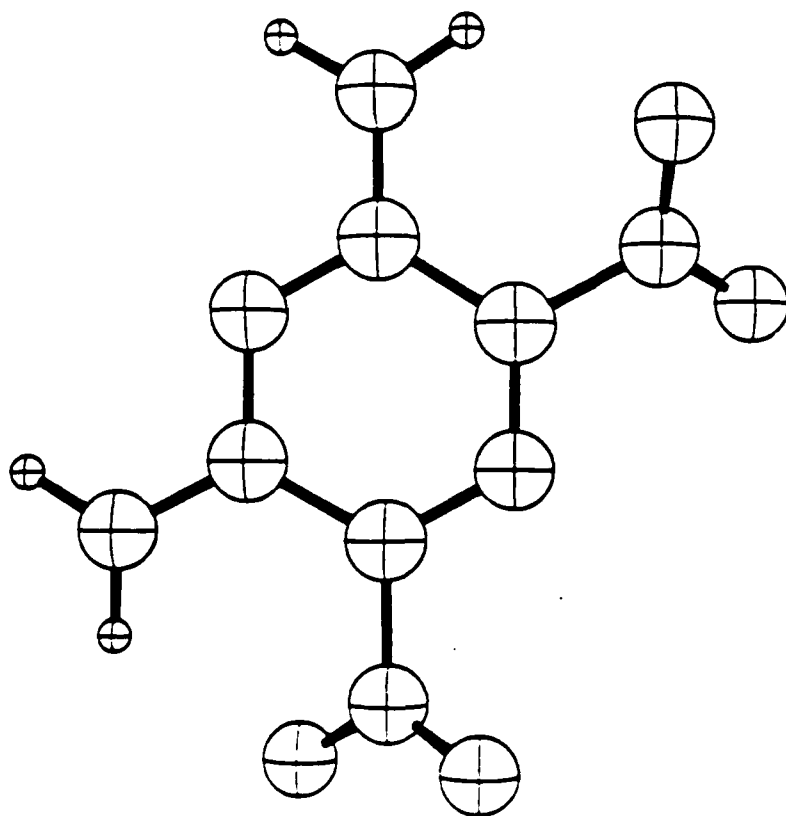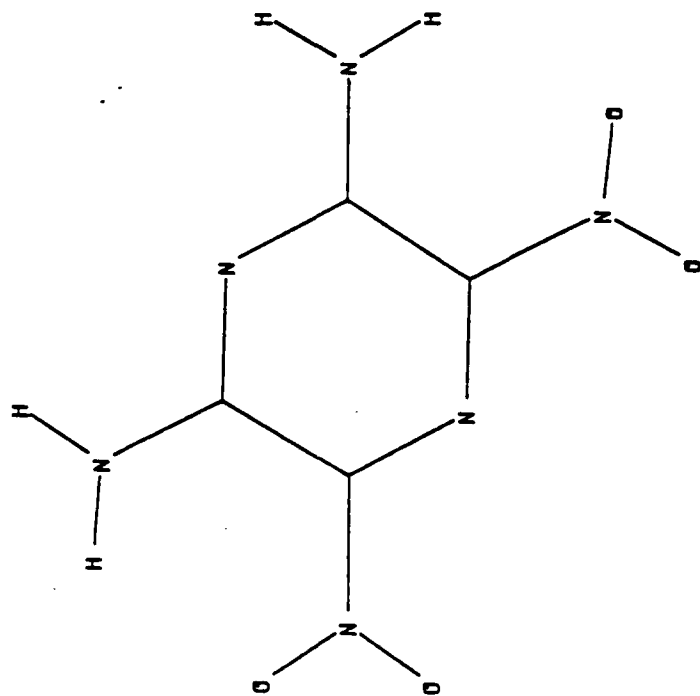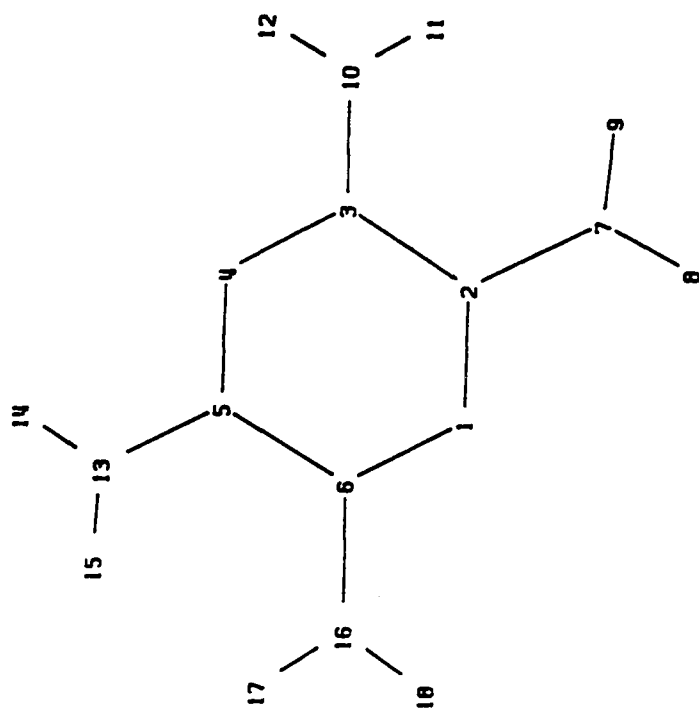
Figure A-1. 2,6-Diamino-3,5-dinitropyrazine [Ref. A-1].

97

C4   H4   N6   O4

AM1
RUN ON HMX/RDX REPLACEMENT 2,6-diamino-3,5-dinitropyrazine (ANANPZ)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	61.157313 KCAL
ELECTRONIC ENERGY	=-14623.069154 EV
CORE-CORE REPULSION	= 11539.618103 EV
DIPOLE	=	7.88306 DEBYE
NO. OF FILLED LEVELS	=	37
IONISATION POTENTIAL	=	9.996250 EV
MOLECULAR WEIGHT	=	200.113
SCF CALCULATIONS	=	8
COMPUTATION TIME	=	129.88 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000
AM1
RUN ON HMX/RDX REPLACEMENT 2,6-diamino-3,5-dinitropyrazine (ANANPZ)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0617
C	1.343492	1	0.000000	0	0.000000	0	1	0	0	-0.2513
C	1.468988	1	121.736580	1	0.000000	0	2	1	0	0.2579
N	1.369061	1	119.145783	1	-1.193982	1	3	2	1	-0.2978
C	1.369654	1	119.533751	1	0.198049	1	4	3	2	0.2584
C	1.468845	1	119.192319	1	1.135374	1	5	4	3	-0.2519
N	1.498269	1	117.501282	1	-179.071970	1	2	1	6	0.5980
O	1.193631	1	120.064598	1	35.283998	1	7	2	1	-0.2917
O	1.205964	1	117.611880	1	-145.726658	1	7	2	1	-0.3930
N	1.360989	1	122.633255	1	-178.665727	1	3	2	1	-0.3258
H	0.995481	1	120.211073	1	-13.136894	1	10	3	2	0.2724
H	0.994008	1	119.961866	1	-178.475286	1	10	3	2	0.2512
N	1.360584	1	118.086386	1	178.626057	1	5	4	3	-0.3263
H	0.994080	1	119.980657	1	3.715424	1	13	5	4	0.2517
H	0.995487	1	120.328373	1	170.316417	1	13	5	4	0.2731
N	1.498107	1	117.529226	1	-179.111820	1	6	1	2	0.5983
O	1.205951	1	117.651891	1	-146.049025	1	16	6	1	-0.3932
O	1.193643	1	120.034007	1	35.053696	1	16	6	1	-0.2918
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C4   H4   N6   O4

MINDO/3
RUN ON HMX/RDX REPLACEMENT 2,6-diamino-3,5-dinitropyrazine (ANANPZ)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-68.528701	KCAL
ELECTRONIC ENERGY	=	-14357.670545	EV
CORE-CORE REPULSION	=	11395.049309	EV
DIPOLE	=	8.84026	DEBYE
NO. OF FILLED LEVELS	=	37	
IONISATION POTENTIAL	=	8.924477	EV
MOLECULAR WEIGHT	=	200.113	
SCF CALCULATIONS	=	77	
COMPUTATION TIME	=	591.44	SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO3 T=36000
MINDO/3
RUN ON HMX/RDX REPLACEMENT 2,6-diamino-3,5-dinitropyrazine (ANANPZ)

Atom											CHARGE
N	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0973
C	1.328469	1	0.000000	0	0.000000	0	1	0	0	-0.3190
C	1.460396	1	116.450692	1	0.000000	0	2	1	0	0.4254
N	1.340126	1	118.419823	1	2.546609	1	3	2	1	-0.3756
C	1.339535	1	123.609756	1	-1.179605	1	4	3	2	0.4250
C	1.460837	1	118.350596	1	-1.463431	1	5	4	3	-0.3175
N	1.416702	1	113.350897	1	177.120488	1	2	1	6	1.1363
O	1.225721	1	115.670221	1	35.488636	1	7	2	1	-0.5701
O	1.231347	1	113.405198	1	-145.328209	1	7	2	1	-0.6118
N	1.327551	1	128.154525	1	-174.418634	1	3	2	1	-0.1443
H	1.013792	1	126.388383	1	-2.381595	1	10	3	2	0.1172
H	1.017255	1	124.439664	1	177.110159	1	10	3	2	0.1047
N	1.327579	1	113.474022	1	175.949975	1	5	4	3	-0.1446
H	1.017197	1	124.438084	1	0.023409	1	13	5	4	0.1049
H	1.013801	1	126.373268	1	-179.572541	1	13	5	4	0.1168
N	1.417183	1	113.349798	1	177.026568	1	6	1	2	1.1360
O	1.231177	1	113.359636	1	-144.107922	1	16	6	1	-0.6110
O	1.225508	1	115.667373	1	36.731590	1	16	6	1	-0.5696
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C4 H4 N6 O4

MNDO
RUN ON HMX/RDX REPLACEMENT 2,6-diamino-3,5-dinitropyrazine (ANANPZ)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	67.266374 KCAL
ELECTRONIC ENERGY	=-14601.178941 EV
CORE-CORE REPULSION	= 11509.097462 EV
DIPOLE	= 7.62639 DEBYE
NO. OF FILLED LEVELS	= 37
IONISATION POTENTIAL	= 10.457755 EV
MOLECULAR WEIGHT	= 200.113
SCF CALCULATIONS	= 14
COMPUTATION TIME	= 200.54 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
 BONDS PRECISE PULAY T=36000
 MNDO
 RUN ON HMX/RDX REPLACEMENT 2,6-diamino-3,5-dinitropyrazine (ANANPZ)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0339
C	1.342622	1	0.000000	0	0.000000	0	1	0	0	-0.1128
C	1.434646	1	122.825757	1	0.000000	0	2	1	0	0.2805
N	1.362569	1	119.330812	1	-0.250182	1	3	2	1	-0.3192
C	1.362678	1	118.953672	1	0.091054	1	4	3	2	0.2809
C	1.434461	1	119.257175	1	0.086632	1	5	4	3	-0.1128
N	1.498423	1	112.993993	1	-179.755242	1	2	1	6	0.5099
O	1.205469	1	119.131269	1	72.079522	1	7	2	1	-0.2860
O	1.210241	1	118.235917	1	-108.841634	1	7	2	1	-0.3327
N	1.386232	1	124.789555	1	-173.445167	1	3	2	1	-0.2535
H	1.003095	1	117.061306	1	-38.354636	1	10	3	2	0.1842
H	1.005103	1	116.219099	1	-172.486174	1	10	3	2	0.1868
N	1.385985	1	115.588806	1	173.966570	1	5	4	3	-0.2537
H	1.005100	1	116.266563	1	14.070415	1	13	5	4	0.1869
H	1.003053	1	117.123404	1	148.274952	1	13	5	4	0.1844
N	1.498814	1	112.962719	1	-179.794351	1	6	1	2	0.5097
O	1.210240	1	118.226559	1	-108.787539	1	16	6	1	-0.3325
O	1.205513	1	119.130027	1	72.119992	1	16	6	1	-0.2862
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

ATNBF.ARC
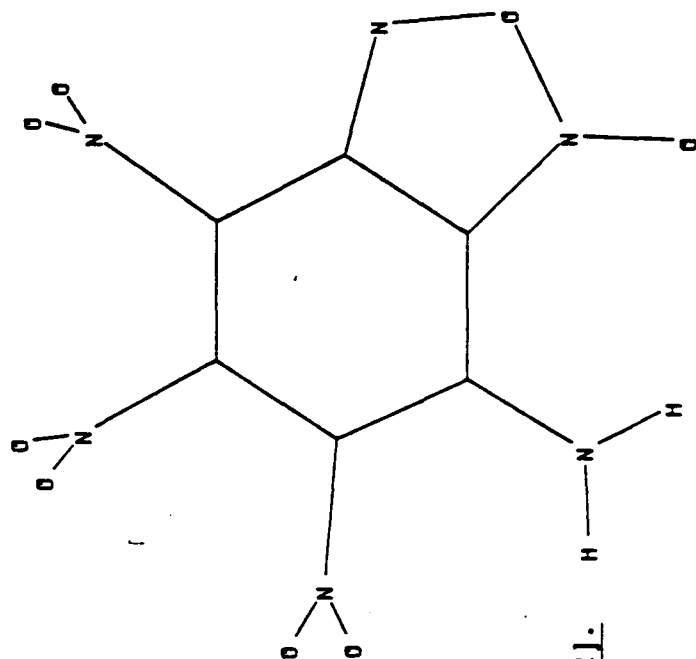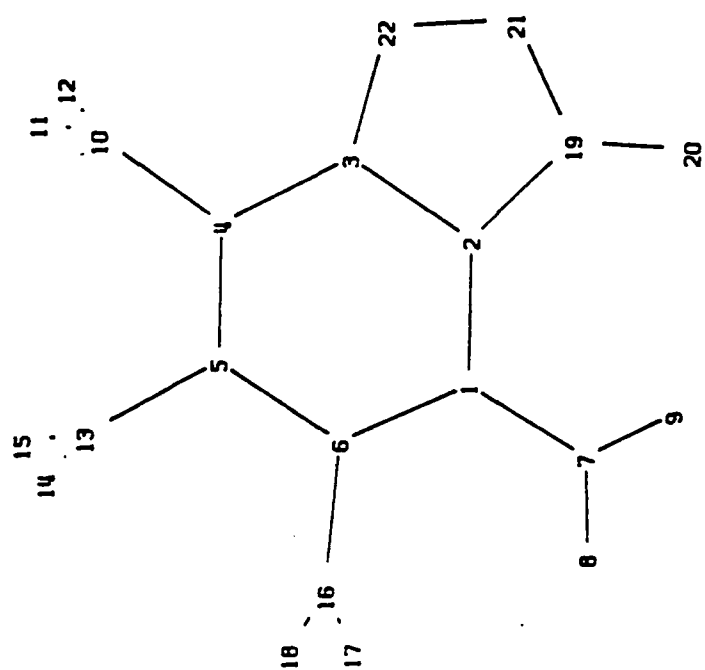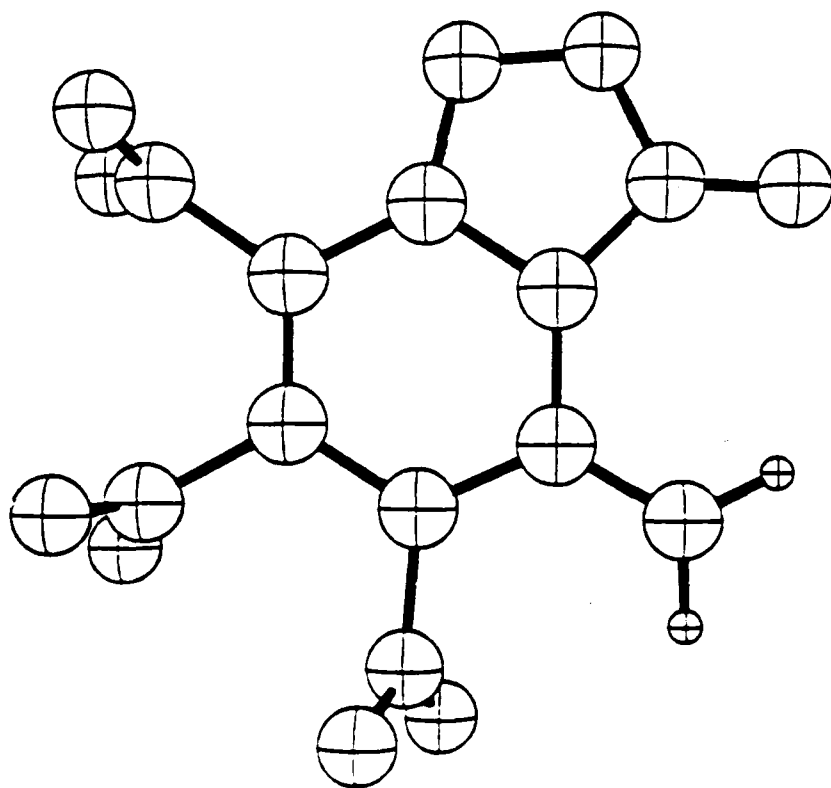
Figure A-2. 7-Amino-4,5,6-trinitrobenzofuroxan [Ref. A-2].

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VERSION   3.00

C6   H2   N6   O8

10-NOV-85

AM1 RUN ON POTENTIAL RDX/HMX REPLACEMENT 7-amino-4,5,6-
trinitrobenzofuroxan (ATNBF)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	147.303189 KCAL
ELECTRONIC ENERGY	=-25784.838674 EV
CORE-CORE REPULSION	= 21201.253618 EV
GRADIENT NORM	=	2.612310
DIPOLE	=	8.90452 DEBYE
NO. OF FILLED LEVELS	=	52
IONISATION POTENTIAL	=	10.409494 EV
MOLECULAR WEIGHT	=	286.117
SCF CALCULATIONS	=	182
COMPUTATION TIME	= 64393.22 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 RESTART
MINDO/3 RUN ON POTENTIAL RDX/HMX REPLACEMENT 7-amino-4,5,6-
trinitrobenzofuroxan (ATNBF)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3247
C	1.437466	1	0.000000	0	0.000000	0	1	0	0	-0.2873
C	1.464487	1	124.235151	1	0.000000	0	2	1	0	0.0461
C	1.433534	1	117.931781	1	-0.916940	1	3	2	1	-0.1526
C	1.383481	1	118.241652	1	1.831631	1	4	3	2	0.1032
C	1.435180	1	123.425741	1	1.257227	1	5	4	3	-0.2984
N	1.346687	1	119.638710	1	178.639779	1	1	2	3	-0.3118
H	0.999931	1	121.305103	1	-175.568998	1	7	1	2	0.2863
H	0.995823	1	120.600682	1	0.619135	1	7	1	2	0.2642
N	1.491805	1	117.671302	1	-177.144878	1	4	3	2	0.5934
O	1.198171	1	118.286311	1	134.170630	1	10	4	3	-0.3251
O	1.195631	1	118.033309	1	-44.768825	1	10	4	3	-0.3007
N	1.518860	1	118.073223	1	-178.049160	1	5	4	3	0.5750
O	1.193649	1	117.384663	1	122.935066	1	13	5	4	-0.2957
O	1.192976	1	117.629842	1	-56.846871	1	13	5	4	-0.2901
N	1.484033	1	119.678461	1	173.551877	1	6	5	4	0.5958
O	1.205398	1	118.662585	1	144.991509	1	16	6	5	-0.3767
O	1.196953	1	119.296833	1	-37.445810	1	16	6	5	-0.3106
N	1.390434	1	131.243835	1	177.926142	1	2	1	6	0.4206
O	1.181697	1	135.263074	1	-1.346691	1	19	2	1	-0.2516
O	1.374458	1	107.311024	1	179.484711	1	19	2	1	-0.0273
N	1.351024	1	108.628938	1	-179.292662	1	3	2	1	0.0186
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

VERSION 3.00

C6 H2 N6 O8

6-NOV-85

MINDO/3 RUN ON POTENTIAL RDX/HMX REPLACEMENT 7-amino-4,5,6-trinitrobenzofuroxan (ATNBF)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-45.691366 KCAL
ELECTRONIC ENERGY	=	-25223.179328 EV
CORE-CORE REPULSION	=	20798.705636 EV
DIPOLE	=	7.08719 DEBYE
NO. OF FILLED LEVELS	=	52
IONISATION POTENTIAL	=	9.443752 EV
MOLECULAR WEIGHT	=	286.117
SCF CALCULATIONS	=	9
COMPUTATION TIME	=	2468.83 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000

MINDO/3 RUN ON POTENTIAL RDX/HMX REPLACEMENT 7-amino-4,5,6-trinitrobenzofuroxan (ATNBF)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.4223
C	1.471272	1	0.000000	0	0.000000	0	1	0	0	-0.3540
C	1.484181	1	120.680162	1	0.000000	0	2	1	0	0.1764
C	1.471260	1	120.088154	1	-0.313053	1	3	2	1	-0.2536
C	1.395892	1	117.897077	1	-1.652646	1	4	3	2	0.0847
C	1.469389	1	122.909592	1	1.245375	1	5	4	3	-0.4126
N	1.325124	1	119.451938	1	-175.180243	1	1	2	3	-0.1246
H	1.014975	1	126.927434	1	177.599085	1	7	1	2	0.1245
H	1.014326	1	125.843746	1	-3.237598	1	7	1	2	0.1342
N	1.439974	1	115.024141	1	178.604237	1	4	3	2	1.1197
O	1.222452	1	113.900310	1	108.470617	1	10	4	3	-0.5520
O	1.222966	1	113.154041	1	-68.815173	1	10	4	3	-0.5481
N	1.451731	1	118.584798	1	-178.850802	1	5	4	3	1.0627
O	1.222684	1	113.133283	1	104.736984	1	13	5	4	-0.5251
O	1.222922	1	113.064494	1	-73.947931	1	13	5	4	-0.5265
N	1.437881	1	119.681072	1	-177.873507	1	6	5	4	1.1328
O	1.224956	1	113.674844	1	110.507009	1	16	6	5	-0.5650

O	1.223791	1	114.348291	1	-71.878010	1	16	6	5	-0.5639
N	1.332513	1	133.590478	1	-177.235421	1	2	1	6	0.9220
O	1.226599	1	130.603787	1	0.161697	1	19	2	1	-0.5436
O	1.358941	1	106.385129	1	179.674832	1	19	2	1	-0.3207
N	1.307913	1	108.161116	1	-179.741571	1	3	2	1	0.1103
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C6 H2 N6 O8

9-NOV-85

MNDO RUN ON POTENTIAL RDX/HMX REPLACEMENT 7-amino-4,5,6-
trinitrobenzofuroxan (ATNBF)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	153.896451	KCAL
ELECTRONIC ENERGY	=-	25618.958121	EV
CORE-CORE REPULSION	=	21021.337764	EV
GRADIENT NORM	=	2.937595	
DIPOLE	=	8.81135	DEBYE
NO. OF FILLED LEVELS	=	52	
IONISATION POTENTIAL	=	10.550230	EV
MOLECULAR WEIGHT	=	286.117	
SCF CALCULATIONS	=	6	
COMPUTATION TIME	=	35161.89	SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 RESTART

MINDO/3 RUN ON POTENTIAL RDX/HMX REPLACEMENT 7-amino-4,5,6-
trinitrobenzofuroxan (ATNBF)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3674
C	1.447278	1	0.000000	0	0.000000	0	1	0	0	-0.2371
C	1.457319	1	122.887176	1	0.000000	0	2	1	0	0.0797
C	1.441426	1	119.677414	1	-0.002676	1	3	2	1	-0.0746
C	1.382455	1	117.643441	1	-1.192354	1	4	3	2	0.1615
C	1.444793	1	122.435905	1	0.980995	1	5	4	3	-0.2408
N	1.364970	1	120.883159	1	-174.729738	1	1	2	3	-0.2874
H	0.999581	1	122.218981	1	-171.729508	1	7	1	2	0.2186
H	0.999266	1	121.253702	1	-15.418418	1	7	1	2	0.2153
N	1.500344	1	118.063758	1	179.072423	1	4	3	2	0.4962

```
0    1.207921  1  118.382367  1   101.950885  1  10  4  3     -0.2961
0    1.206417  1  118.484530  1   -77.228601  1  10  4  3     -0.2810
N    1.517380  1  119.016248  1  -178.888540  1   5  4  3      0.4590
0    1.206853  1  118.303827  1   102.736224  1  13  5  4     -0.2768
0    1.206586  1  118.322539  1   -76.692473  1  13  5  4     -0.2733
N    1.499972  1  118.039721  1  -179.256836  1   6  5  4      0.4860
0    1.210037  1  118.665603  1   107.405192  1  16  6  5     -0.3134
0    1.208046  1  119.084169  1   -73.967684  1  16  6  5     -0.2946
N    1.403183  1  134.530514  1  -178.717182  1   2  1  6      0.3591
0    1.197313  1  133.023891  1     0.543588  1  19  2  1     -0.2351
0    1.349177  1  108.736301  1   179.806757  1  19  2  1      0.0249
N    1.349260  1  108.516159  1  -179.867372  1   3  2  1     -0.0575
0    0.000000  0    0.000000  0     0.000000  0   0  0  0
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BTF.ARC
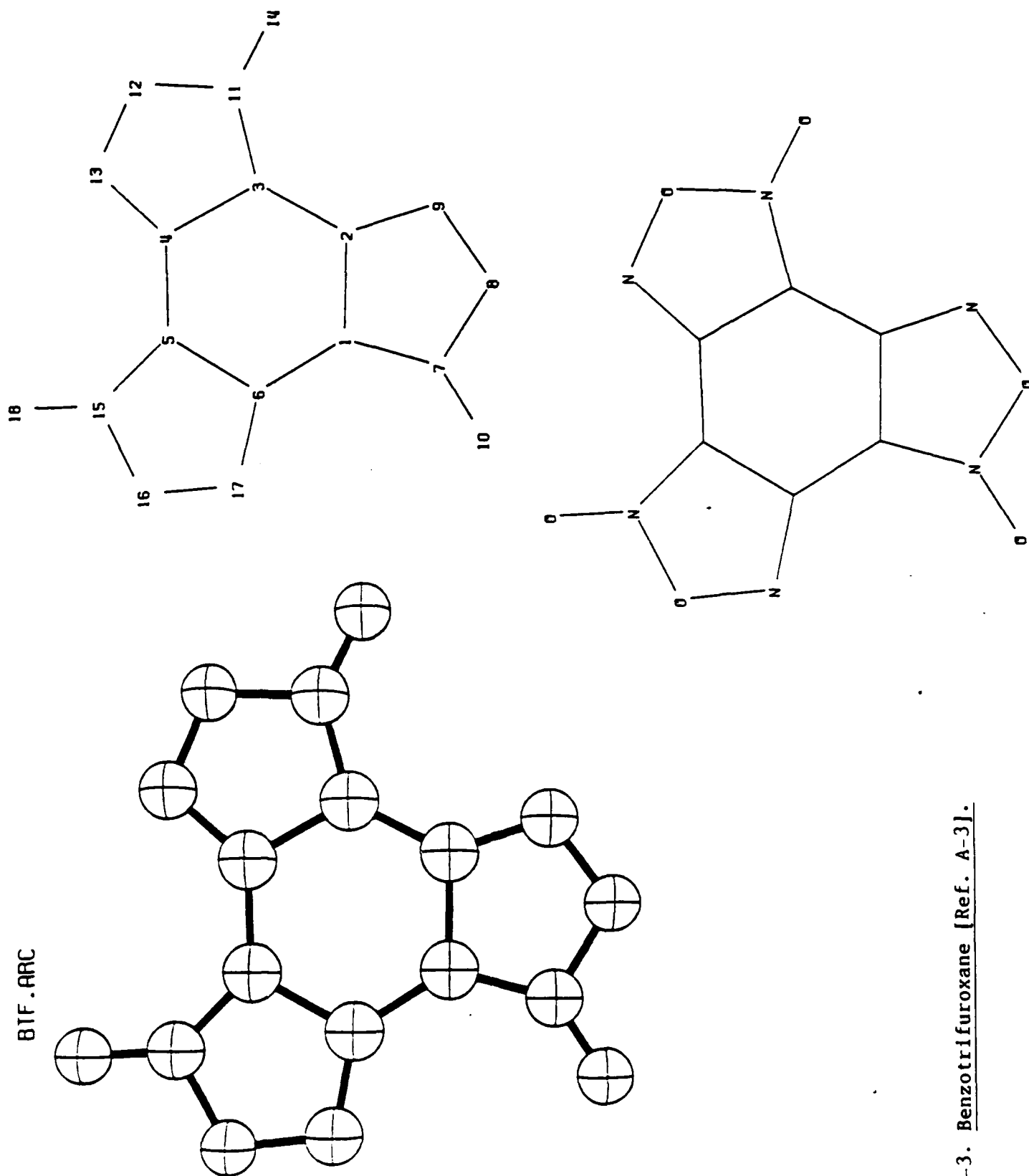
Figure A-3. Benzotrifuroxane [Ref. A-3].

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SUMMARY OF   AM1   CALCULATION

VERSION 3.00

C6   N6   06

9-NOV-85
RUN ON POTENTIAL RDX/HMX REPLACEMENT benzotrifuroxane (BTF)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	297.385482 KCAL
ELECTRONIC ENERGY	=-	20387.545699 EV
CORE-CORE REPULSION	=	16475.144562 EV
DIPOLE	=	0.00440 DEBYE
NO. OF FILLED LEVELS	=	45
IONISATION POTENTIAL	=	10.580912 EV
MOLECULAR WEIGHT	=	252.103
SCF CALCULATIONS	=	291
COMPUTATION TIME	=	29378.20 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000
AM1
RUN ON POTENTIAL RDX/HMX REPLACEMENT benzotrifuroxane (BTF)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.2192
C	1.481954	1	0.000000	0	0.000000	0	1	0	0	0.0708
C	1.420559	1	117.595637	1	0.000000	0	2	1	0	-0.2191
C	1.481878	1	122.315997	1	-0.221185	1	3	2	1	0.0706
C	1.420463	1	117.734175	1	0.379512	1	4	3	2	-0.2194
C	1.481797	1	122.304180	1	-0.266544	1	5	4	3	0.0707
N	1.377758	1	104.770408	1	179.985904	1	1	2	3	0.4339
O	1.400030	1	106.780036	1	0.019432	1	7	1	2	-0.0670
N	1.343492	1	133.577643	1	179.736001	1	2	3	4	0.0075
O	1.177691	1	137.894007	1	180.024045	1	7	1	2	-0.2259
N	1.377499	1	104.817740	1	179.929670	1	3	4	5	0.4341
O	1.400268	1	106.748170	1	0.126886	1	11	3	4	-0.0671
N	1.343606	1	133.474317	1	179.684753	1	4	5	6	0.0073
O	1.177681	1	137.917886	1	179.791858	1	11	3	4	-0.2259
N	1.377450	1	104.846998	1	179.947685	1	5	6	1	0.4343
O	1.400452	1	106.710066	1	-0.001001	1	15	5	6	-0.0674
N	1.343519	1	133.600331	1	-179.915288	1	6	1	2	0.0076
O	1.177541	1	137.943152	1	180.016210	1	15	5	6	-0.2257
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C6 N6 O6

8-NOV-85

MINDO/3
RUN ON POTENTIAL RDX/HMX REPLACEMENT benzotrifuroxane (BTF)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-26.171648 KCAL
ELECTRONIC ENERGY	=-19951.639989 EV
CORE-CORE REPULSION	= 16176.846704 EV
DIPOLE	=	0.00285 DEBYE
NO. OF FILLED LEVELS	=	45
IONISATION POTENTIAL	=	9.541911 EV
MOLECULAR WEIGHT	=	252.103
SCF CALCULATIONS	=	8
COMPUTATION TIME	=	1667.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000
MINDO/3
RUN ON POTENTIAL RDX/HMX REPLACEMENT benzotrifuroxane (BTF)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.2999
C	1.491066	1	0.000000	0	0.000000	0	1	0	0	0.1801
C	1.467367	1	118.352039	1	0.000000	0	2	1	0	-0.2999
C	1.491090	1	121.646589	1	0.068969	1	3	2	1	0.1801
C	1.467383	1	118.355237	1	-0.121379	1	4	3	2	-0.2998
C	1.491008	1	121.641463	1	0.108037	1	5	4	3	0.1801
N	1.315871	1	106.777095	1	180.003887	1	1	2	3	0.9049
O	1.374763	1	105.684883	1	-0.007060	1	7	1	2	-0.3561
N	1.302668	1	133.796506	1	180.066970	1	2	3	4	0.1218
O	1.228019	1	131.291917	1	179.997047	1	7	1	2	-0.5508
N	1.315865	1	106.773475	1	179.968100	1	3	4	5	0.9049
O	1.374756	1	105.689993	1	-0.017620	1	11	3	4	-0.3561
N	1.302666	1	133.793270	1	180.042030	1	4	5	6	0.1218
O	1.228025	1	131.295057	1	179.999845	1	11	3	4	-0.5508
N	1.315834	1	106.794770	1	179.991622	1	5	6	1	0.9049
O	1.374825	1	105.669467	1	-0.010250	1	15	5	6	-0.3562
N	1.302682	1	133.798681	1	179.965611	1	6	1	2	0.1219
O	1.228002	1	131.306818	1	180.003147	1	15	5	6	-0.5508
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

VERSION 3.00

C6 N6 O6

8-NOV-85

MNDO
RUN ON POTENTIAL RDX/HMX REPLACEMENT benzofuroxane (BTF)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	197.020831 KCAL
ELECTRONIC ENERGY	=	-20429.345901 EV
CORE-CORE REPULSION	=	16502.829090 EV
DIPOLE	=	0.00131 DEBYE
NO. OF FILLED LEVELS	=	45
IONISATION POTENTIAL	=	10.557442 EV
MOLECULAR WEIGHT	=	252.103
SCF CALCULATIONS	=	239
COMPUTATION TIME	=	21987.01 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000
MNDO
RUN ON POTENTIAL RDX/HMX REPLACEMENT benzotrifuroxane (BTF)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1903
C	1.470349	1	0.000000	0	0.000000	0	1	0	0	0.1208
C	1.431027	1	117.962872	1	0.000000	0	2	1	0	-0.1905
C	1.470248	1	121.968778	1	-0.121380	1	3	2	1	0.1207
C	1.430586	1	118.028406	1	0.184239	1	4	3	2	-0.1904
C	1.470240	1	122.043842	1	-0.127457	1	5	4	3	0.1207
N	1.388551	1	103.214758	1	180.010492	1	1	2	3	0.3694
O	1.360730	1	108.347344	1	-0.009087	1	7	1	2	-0.0117
N	1.342159	1	133.892485	1	179.862130	1	2	3	4	-0.0623
O	1.196041	1	133.648718	1	179.995514	1	7	1	2	-0.2259
N	1.388419	1	103.271887	1	180.045125	1	3	4	5	0.3697
O	1.360838	1	108.298286	1	0.039198	1	11	3	4	-0.0118
N	1.342202	1	133.867271	1	179.975444	1	4	5	6	-0.0624
O	1.195974	1	133.674662	1	180.022017	1	11	3	4	-0.2259
N	1.388624	1	103.215166	1	180.009665	1	5	6	1	0.3695
O	1.360774	1	108.334099	1	0.006625	1	15	5	6	-0.0117
N	1.342031	1	133.939014	1	180.049543	1	6	1	2	-0.0622
O	1.195987	1	133.658045	1	179.994947	1	15	5	6	-0.2258
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

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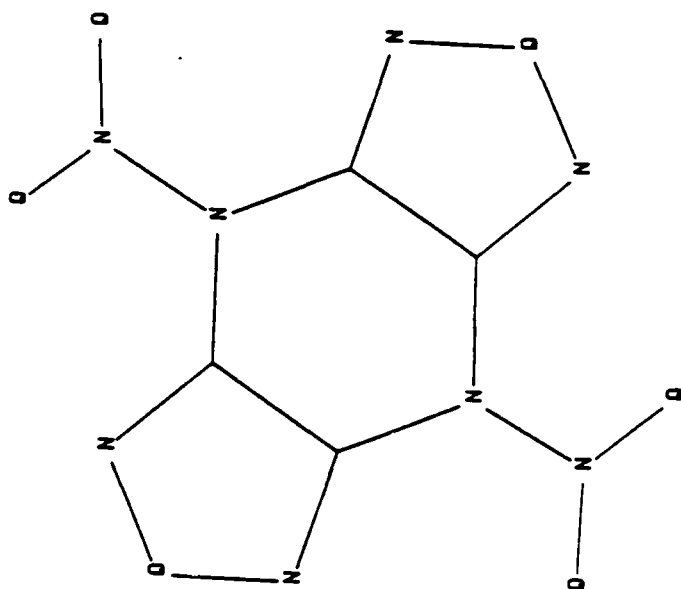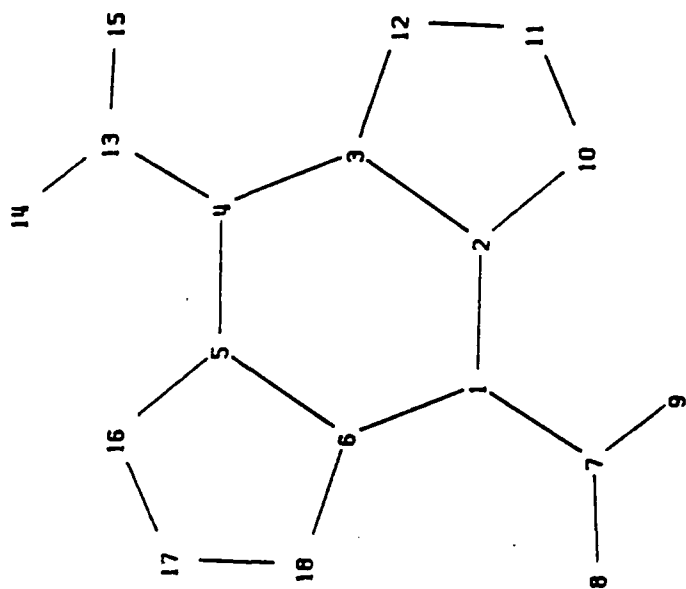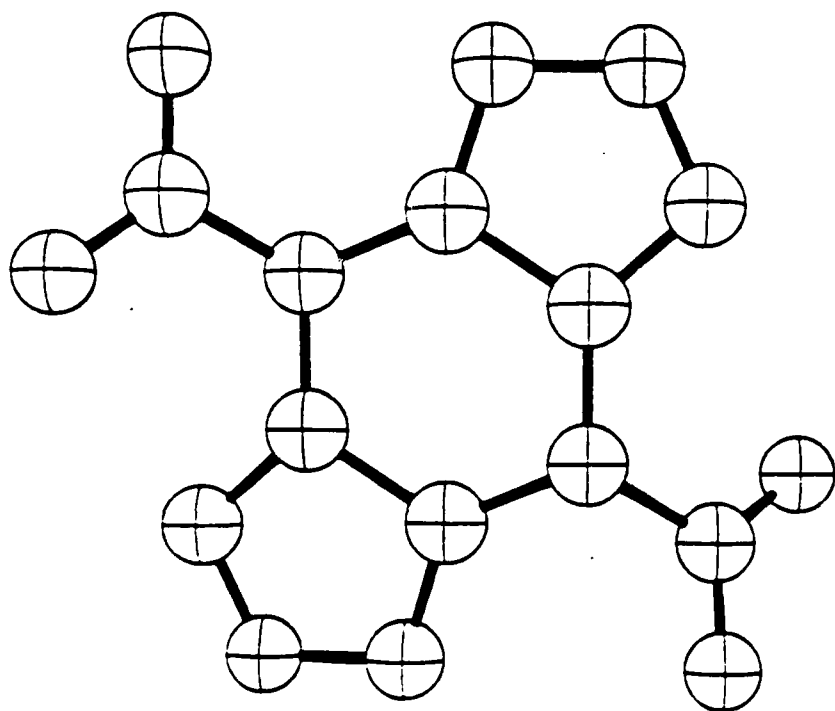
Figure 'A-4. 1,4-Dinitro-[3,4-b],[3,4-e]difurazanopiperazine [Ref. A-4].

SUMMARY OF   AM1   CALCULATION

C4   N8   O6

RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,4-dinitro-[3,4-b],[3,4,-e]-difurazanopiperazine (DNDFP)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	292.439136 KCAL
ELECTRONIC ENERGY	=-21461.552077 EV
CORE-CORE REPULSION	= 17390.773149 EV
GRADIENT NORM	=	2.869061
DIPOLE	=	0.10693 DEBYE
NO. OF FILLED LEVELS	=	46
IONISATION POTENTIAL	=	11.050266 EV
MOLECULAR WEIGHT	=	256.094
SCF CALCULATIONS	=	310
COMPUTATION TIME	=	5163.83 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 AM1
RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,4-dinitro-[3,4-b],[3,4-e]-difurazanopiperazine (DNDFP)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1406
C	1.416374	1	0.000000	0	0.000000	0	1	0	0	-0.0552
C	1.514409	1	123.620887	1	0.000000	0	2	1	0	-0.0452
N	1.415513	1	123.347683	1	-7.868281	1	3	2	1	-0.1565
C	1.415035	1	112.526273	1	0.362932	1	4	3	2	-0.0445
C	1.510790	1	123.792000	1	-0.460111	1	5	4	3	-0.0534
N	1.467521	1	118.969360	1	155.881878	1	1	2	3	0.6291
O	1.187360	1	115.225255	1	164.725976	1	7	1	2	-0.2407
O	1.190175	1	118.071566	1	-12.093072	1	7	1	2	-0.2721
N	1.352507	1	105.744544	1	177.275480	1	2	3	4	0.0623
O	1.332089	1	106.652740	1	0.078092	1	10	2	3	0.0027
N	1.352423	1	130.811854	1	176.805489	1	3	4	5	0.0712
N	1.457004	1	119.089961	1	-146.000338	1	4	5	6	0.6356
O	1.190820	1	117.319564	1	-3.356988	1	13	4	5	-0.2711
O	1.189115	1	116.263365	1	-179.759482	1	13	4	5	-0.2536
N	1.353408	1	105.712342	1	-176.874297	1	5	6	1	0.0731
O	1.330714	1	106.684635	1	0.086024	1	16	5	6	0.0043
N	1.352663	1	130.633165	1	169.775797	1	6	1	2	0.0545
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

VERSION   3.00

C4   N8   06

RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,4-dinitro-[3,4-b],[3,4-e]-difurazanopiperazine (DNDFP)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-64.052245	KCAL
ELECTRONIC ENERGY	=	-21210.450083	EV
CORE-CORE REPULSION	=	17302.954770	EV
DIPOLE	=	0.05184	DEBYE
NO. OF FILLED LEVELS	=	46	
IONISATION POTENTIAL	=	9.332637	EV
MOLECULAR WEIGHT	=	256.094	
SCF CALCULATIONS	=	114	
COMPUTATION TIME	=	931.85	SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 MINDO3
RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,4-dinitro-[3,4-b],[3,4-e]-difurazanopiperazine (DNDFP)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1992
C	1.413731	1	0.000000	0	0.000000	0	1	0	0	0.0734
C	1.496237	1	122.949181	1	0.000000	0	2	1	0	0.0734
N	1.413674	1	122.955869	1	-0.322943	1	3	2	1	-0.1993
C	1.413773	1	114.074038	1	-0.551727	1	4	3	2	0.0733
C	1.496492	1	122.984438	1	0.689977	1	5	4	3	0.0734
N	1.313085	1	122.954634	1	-179.009399	1	1	2	3	1.1599
O	1.229850	1	114.332957	1	179.972776	1	7	1	2	-0.5773
O	1.229771	1	114.331718	1	-0.033978	1	7	1	2	-0.5773
N	1.304205	1	107.358998	1	179.836496	1	2	3	4	0.1434
O	1.340692	1	104.622087	1	-0.021480	1	10	2	3	-0.2396
N	1.304227	1	129.688943	1	179.214420	1	3	4	5	0.1434
N	1.312919	1	122.968757	1	-179.256176	1	4	5	6	1.1602
O	1.229710	1	114.334110	1	-0.056598	1	13	4	5	-0.5773
O	1.229708	1	114.327352	1	179.947205	1	13	4	5	-0.5774
N	1.304199	1	107.359891	1	179.781968	1	5	6	1	0.1433
O	1.340650	1	104.623327	1	0.065701	1	16	5	6	-0.2396
N	1.304194	1	129.749686	1	178.856078	1	6	1	2	0.1434
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF   MNDO   CALCULATION

VERSION 3.00

C4 N8 06

RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,4-dinitro-[3,4-b],[3,4-e]-
difurazanopiperazine (DNDFP)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   187.845094 KCAL
ELECTRONIC ENERGY   =-21567.131638 EV
CORE-CORE REPULSION   = 17481.076344 EV
DIPOLE   =   0.40216 DEBYE
NO. OF FILLED LEVELS   =   46
IONISATION POTENTIAL   =   11.398606 EV
MOLECULAR WEIGHT   =   256.094
SCF CALCULATIONS   =   862
COMPUTATION TIME   = 16243.79 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 SHIFT=30
RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,4-dinitro-[3,4-b],[3,4-e]-
difurazanopipereazine (DNDFP)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1298
C	1.422216	1	0.000000	0	0.000000	0	1	0	0	-0.0016
C	1.468212	1	125.334204	1	0.000000	0	2	1	0	-0.0002
N	1.421958	1	125.269258	1	0.127069	1	3	2	1	-0.1315
C	1.422017	1	108.371301	1	11.319154	1	4	3	2	-0.0003
C	1.467924	1	125.246610	1	-11.292083	1	5	4	3	-0.0015
N	1.462943	1	116.431193	1	-144.982344	1	1	2	3	0.5661
O	1.193422	1	114.354623	1	-114.940407	1	7	1	2	-0.1958
O	1.201971	1	118.505318	1	65.050691	1	7	1	2	-0.2814
N	1.346667	1	105.712719	1	173.770562	1	2	3	4	-0.0029
O	1.305679	1	106.956981	1	0.600318	1	10	2	3	0.0492
N	1.346607	1	128.658680	1	-176.358863	1	3	4	5	-0.0030
N	1.462595	1	116.450686	1	-144.917757	1	4	5	6	0.5667
O	1.201884	1	118.480212	1	65.592194	1	13	4	5	-0.2813
O	1.193316	1	114.363661	1	-114.477826	1	13	4	5	-0.1958
N	1.346667	1	105.744711	1	173.622563	1	5	6	1	-0.0030
O	1.305741	1	106.936464	1	0.575911	1	16	5	6	0.0491
N	1.346772	1	128.558831	1	-176.311223	1	6	1	2	-0.0028
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

113
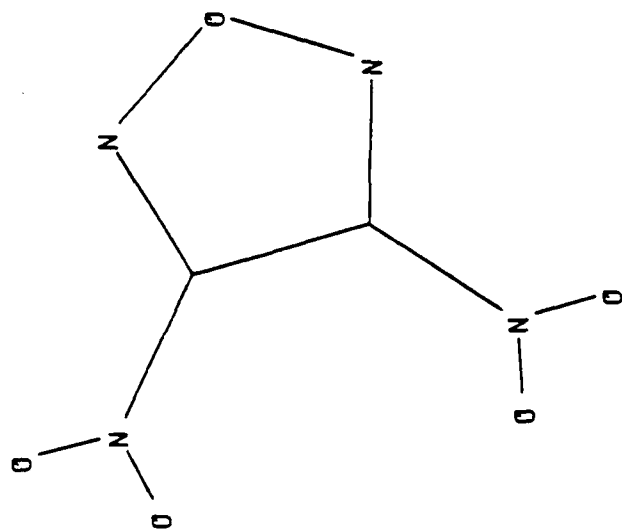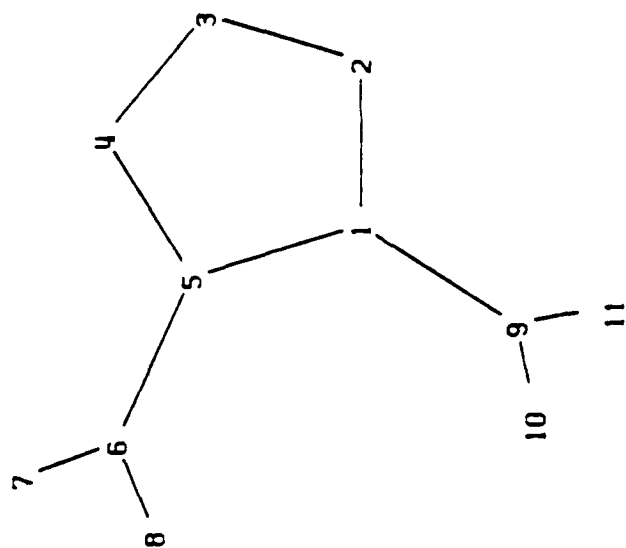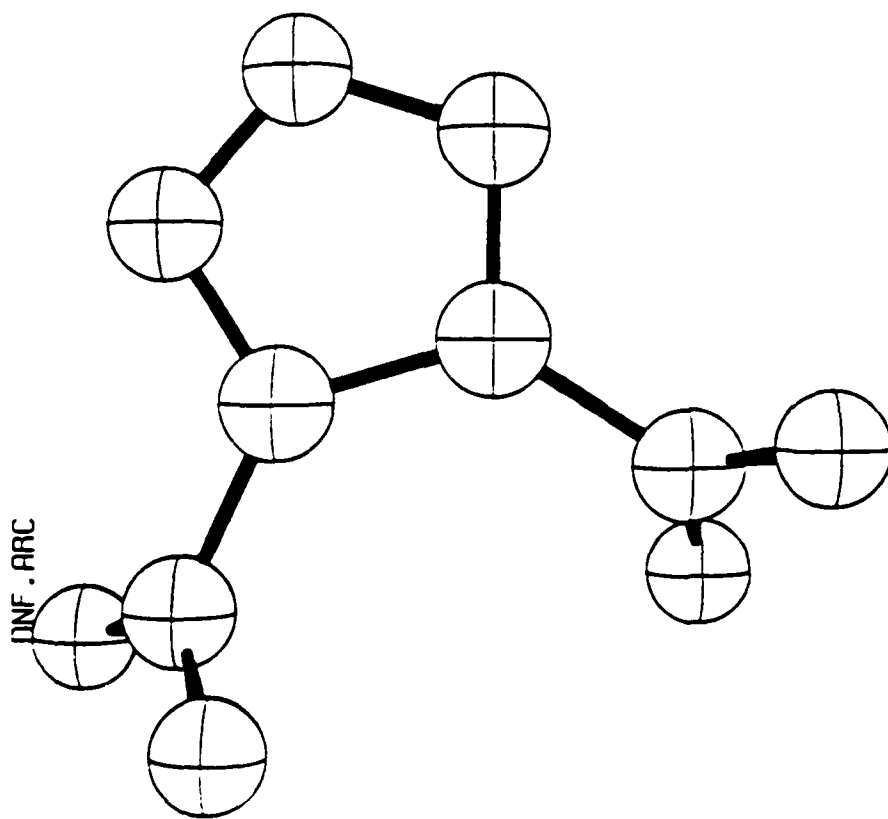
Figure A-5. Dinitrofurazane [Ref. A-4].

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C2   N4   O5

AM1
RUN ON POTENTIAL RDX/HMX REPLACEMENT dinitrofurazane (DNF)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	120.768461 KCAL
ELECTRONIC ENERGY	=	-10594.886597 EV
CORE-CORE REPULSION	=	7921.029107 EV
DIPOLE	=	2.47947 DEBYE
NO. OF FILLED LEVELS	=	29
IONISATION POTENTIAL	=	13.109989 EV
MOLECULAR WEIGHT	=	160.046
SCF CALCULATIONS	=	163
COMPUTATION TIME	=	540.63 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 AM1
AM1
RUN ON POTENTIAL RDX/HMX REPLACEMENT dinitrofurazane (DNF)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1611
N	1.350270	1	0.000000	0	0.000000	0	1	0	0	0.1009
O	1.329875	1	106.549211	1	0.000000	0	2	1	0	0.0187
N	1.329206	1	114.697266	1	0.116907	1	3	2	1	0.1039
C	1.489364	1	106.109536	1	-0.130963	1	1	2	3	-0.1637
N	1.486539	1	128.603566	1	178.904401	1	5	4	3	0.6182
O	1.192361	1	118.397510	1	34.692254	1	6	5	4	-0.2763
O	1.194880	1	116.634810	1	-145.114061	1	6	5	4	-0.2929
N	1.487143	1	125.340496	1	-178.877386	1	1	5	4	0.6189
O	1.194551	1	116.638750	1	39.452494	1	9	1	5	-0.2899
O	1.192335	1	118.271326	1	-140.630035	1	9	1	5	-0.2766
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION   3.00

C2   N4   O5

MINDO/3
RUN ON POTENTIAL RDX/HMX REPLACEMENT dinitrofurazane (DNF)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED


```
        HEAT OF FORMATION       =    -39.048794 KCAL
        ELECTRONIC ENERGY       =-10294.572888 EV
        CORE-CORE REPULSION     =   7721.215361 EV
        DIPOLE                  =       3.04780 DEBYE
        NO. OF FILLED LEVELS    =     29
        IONISATION POTENTIAL    =     10.731621 EV
        MOLECULAR WEIGHT        =    160.046
        SCF CALCULATIONS        =      9
        COMPUTATION TIME        =     48.34 SECONDS
```


```
        FINAL GEOMETRY OBTAINED                                    CHARGE
        BONDS PRECISE PULAY T=36000 MINDO3
        MINDO/3
        RUN ON POTENTIAL RDX/HMX REPLACEMENT dinitrofurazane (DNF)
  C   0.000000 0    0.000000 0    0.000000 0  0 0 0      -0.1366
  N   1.310874 1    0.000000 0    0.000000 0  1 0 0       0.1967
  O   1.327470 1  106.583354 1    0.000000 0  2 1 0      -0.1926
  N   1.326791 1  114.000615 1   -0.055810 1  3 2 1       0.1981
  C   1.486096 1  106.417216 1    0.166057 1  1 2 3      -0.1380
  N   1.426030 1  122.371270 1  177.819808 1  5 4 3       1.1269
  O   1.221519 1  113.691332 1   57.306475 1  6 5 4      -0.5413
  O   1.222709 1  112.883807 1 -121.335254 1  6 5 4      -0.5496
  N   1.426101 1  131.186961 1 -177.704059 1  1 5 4       1.1269
  O   1.222661 1  112.883210 1   56.736591 1  9 1 5      -0.5494
  O   1.221447 1  113.666661 1 -124.630715 1  9 1 5      -0.5410
  O   0.000000 0    0.000000 0    0.000000 0  0 0 0
```


SUMMARY OF MNDO   CALCULATION

VERSION 3.00

C2 N4 O5

MNDO
RUN ON POTENTIAL RDX/HMX REPLACEMENT dinitrofurazane (DNF)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!

SCF FIELD WAS ACHIEVED

```
        HEAT OF FORMATION        =      96.092569 KCAL
        ELECTRONIC ENERGY        =-10519.292922 EV
        CORE-CORE REPULSION      =  7835.457018 EV
        GRADIENT NORM            =     46.830906
        DIPOLE                   =      2.43002 DEBYE
        NO. OF FILLED LEVELS     =     29
        IONISATION POTENTIAL     =     12.663287 EV
        MOLECULAR WEIGHT         =    160.046
        SCF CALCULATIONS         =     36
        COMPUTATION TIME         =    159.73 SECONDS
```

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000
MNDO
RUN ON POTENTIAL RDX/HMX REPLACEMENT dinitrofurazane (DNF)

```
C   0.000000  0    0.000000  0    0.000000  0  0  0  0    -0.0421
N   1.334903  1    0.000000  0    0.000000  0  1  0  0     0.0305
O   1.323448  1  106.730895  1    0.000000  0  2  1  0     0.0550
N   1.298248  1  114.058389  1   -0.472501  1  3  2  1     0.0414
C   1.456184  1  106.546351  1    0.806690  1  1  2  3    -0.0602
N   1.474884  1  123.130251  1  178.992285  1  5  4  3     0.5268
O   1.205975  1  118.315139  1   57.607013  1  6  5  4    -0.2583
O   1.208422  1  117.682802  1 -122.647687  1  6  5  4    -0.2842
N   1.494451  1  130.652302  1 -178.859494  1  1  5  4     0.5287
O   1.204661  1  117.524833  1   56.172420  1  9  1  5    -0.2807
O   1.202238  1  118.229577  1 -123.382976  1  9  1  5    -0.2568
O   0.000000  0    0.000000  0    0.000000  0  0  0  0
```

MDDCP.ARC
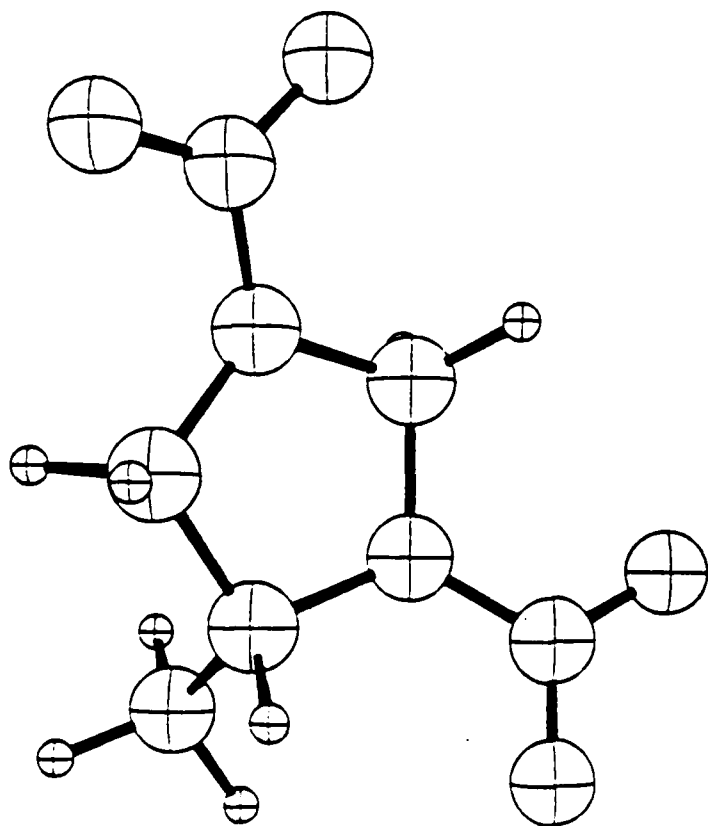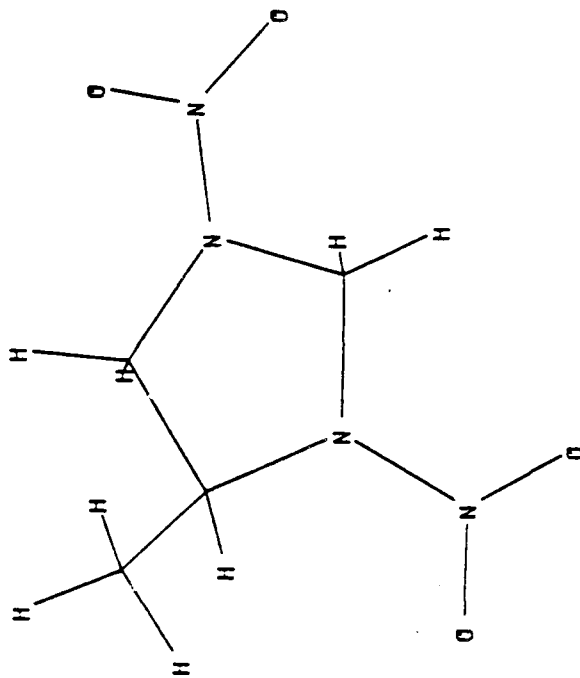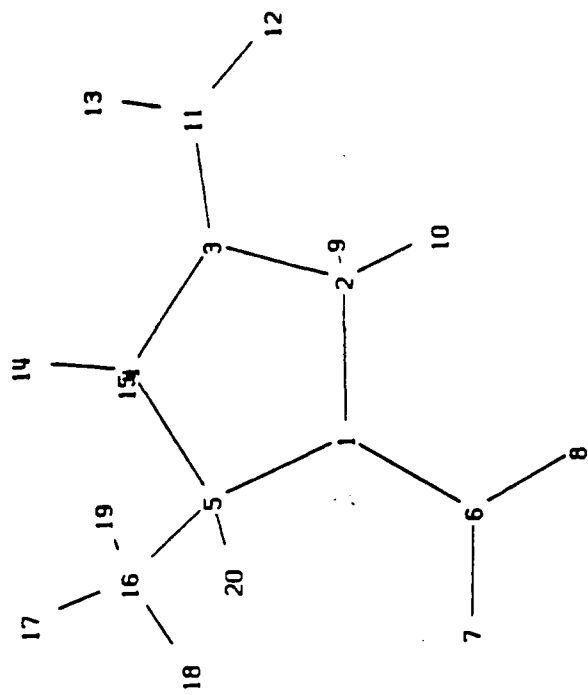
Figure A-6. 4-Methyl-1,3-dinitro-1,3-diazacyclopentane
[Ref. A-5].

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C4   H8   N4   O4

RUN ON HMX/RDX REPLACEMENT 4-methyl-1,3-dinitro-1,3-diazacyclopentane (MDDCP)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	60.700917 KCAL
ELECTRONIC ENERGY	=	-13097.383982 EV
CORE-CORE REPULSION	=	10373.905760 EV
GRADIENT NORM	=	5540.281295
DIPOLE	=	4.88088 DEBYE
NO. OF FILLED LEVELS	=	34
IONISATION POTENTIAL	=	11.554860 EV
MOLECULAR WEIGHT	=	176.132
SCF CALCULATIONS	=	342
COMPUTATION TIME	=	2524.18 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000
RUN ON HMX/RDX REPLACEMENT 4-methyl-1,3-dinitro-1,3-diazacyclopentane
(MDDCP)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.2550
C	1.483947	1	0.000000	0	0.000000	0	1	0	0	-0.0206
N	1.487190	1	109.846364	1	0.000000	0	2	1	0	-0.2475
C	1.476844	1	106.516083	1	-16.268266	1	3	2	1	-0.1161
C	1.559904	1	107.845570	1	8.647526	1	4	3	2	-0.0468
N	1.418495	1	117.355265	1	-116.112621	1	1	2	3	0.5943
O	1.200816	1	118.081326	1	159.522270	1	6	1	2	-0.3393
O	1.200996	1	117.947421	1	-25.969746	1	6	1	2	-0.3412
H	1.132523	1	105.104340	1	96.338821	1	2	3	4	0.1652
H	1.132702	1	113.305576	1	-144.374415	1	2	3	4	0.1833
N	1.421807	1	116.997240	1	117.226403	1	3	2	1	0.5900
O	1.200289	1	117.600051	1	33.720635	1	11	3	2	-0.3346
O	1.201137	1	118.365512	1	-151.919451	1	11	3	2	-0.3445
H	1.124447	1	105.945330	1	-109.796197	1	4	3	2	0.1403
H	1.124494	1	113.194443	1	131.451637	1	4	3	2	0.1445
C	1.520298	1	110.741527	1	-119.431568	1	5	4	3	-0.2072
H	1.117280	1	108.414571	1	-60.537422	1	16	5	4	0.0926
H	1.117057	1	110.401318	1	-179.696497	1	16	5	4	0.1078
H	1.116329	1	111.520924	1	59.346556	1	16	5	4	0.0923
H	1.130705	1	109.383122	1	121.476026	1	5	4	3	0.1424
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C4 H8 N4 O4

RUN ON HMX/RDX REPLACEMENT 4-methyl-1,3-dinitro-1,3-diazacyclopentane (MDDCP)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   -40.378780 KCAL
ELECTRONIC ENERGY   =-12732.175960 EV
CORE-CORE REPULSION   = 10096.538242 EV
DIPOLE   =   3.33153 DEBYE
NO. OF FILLED LEVELS   =   34
IONISATION POTENTIAL   =   10.477410 EV
MOLECULAR WEIGHT   =   176.132
SCF CALCULATIONS   =   71
COMPUTATION TIME   =   317.35 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO3 T=36000
RUN ON HMX/RDX REPLACEMENT 4-methyl-1,3-dinitro-1,3-diazacyclopentane
(MDDCP)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.3241
C	1.454065	1	0.000000	0	0.000000	0	1	0	0	0.3059
N	1.451091	1	104.440389	1	0.000000	0	2	1	0	-0.3069
C	1.459663	1	111.323748	1	-7.862904	1	3	2	1	0.1613
C	1.526612	1	106.947142	1	-1.768081	1	4	3	2	0.1752
N	1.312494	1	122.989044	1	-161.774122	1	1	2	3	1.1891
O	1.229323	1	114.940988	1	171.855737	1	6	1	2	-0.5881
O	1.229609	1	114.682803	1	-8.466105	1	6	1	2	-0.5864
H	1.135225	1	111.943232	1	112.864884	1	2	3	4	-0.0265
H	1.131316	1	112.106840	1	-130.653128	1	2	3	4	-0.0043
N	1.312684	1	124.611773	1	172.503440	1	3	2	1	1.1882
O	1.229174	1	114.606540	1	2.352913	1	11	3	2	-0.5850
O	1.228992	1	114.629065	1	-177.814709	1	11	3	2	-0.5820
H	1.125858	1	112.641286	1	-124.358253	1	4	3	2	-0.0152
H	1.125650	1	112.918951	1	120.060692	1	4	3	2	-0.0117
C	1.514580	1	116.613935	1	-118.400520	1	5	4	3	0.0246
H	1.112646	1	109.962516	1	-51.495242	1	16	5	4	-0.0013
H	1.108631	1	115.820554	1	-169.411482	1	16	5	4	0.0199
H	1.111712	1	115.108526	1	66.716261	1	16	5	4	-0.0107
H	1.134556	1	105.190983	1	125.821903	1	5	4	3	-0.0222

0   0.000000 0   0.000000 0   0.000000 0   0   0   0

SUMMARY OF   MNDO   CALCULATION

VERSION   3.00

C4   H8   N4   O4

RUN ON HMX/RDX REPLACEMENT 4-methyl-1,3-dinitro-1,3-diazacyclopentane
(MDDCP)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	53.438592 KCAL
ELECTRONIC ENERGY	=-12949.504743 EV
CORE-CORE REPULSION	= 10215.123791 EV
DIPOLE	=	3.24119 DEBYE
NO. OF FILLED LEVELS	=	34
IONISATION POTENTIAL	=	11.618736 EV
MOLECULAR WEIGHT	=	176.132
SCF CALCULATIONS	=	388
COMPUTATION TIME	=	2258.64 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000
RUN ON HMX/RDX REPLACEMENT 4-methyl-1,3-dinitro-1,3-diazacyclopentane
(MDDCP)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.3985
C	1.487492	1	0.000000	0	0.000000	0	1	0	0	0.3343
N	1.484643	1	103.255104	1	0.000000	0	2	1	0	-0.4299
C	1.481186	1	113.445519	1	-0.398712	1	3	2	1	0.1577
C	1.557501	1	105.022436	1	-5.471678	1	4	3	2	0.0979
N	1.394775	1	119.599168	1	-145.357396	1	1	2	3	0.5981
O	1.208692	1	118.801881	1	160.012087	1	6	1	2	-0.3281
O	1.209250	1	117.616879	1	-25.047418	1	6	1	2	-0.3250
H	1.121690	1	109.392531	1	114.995651	1	2	3	4	0.0599
H	1.118949	1	112.651046	1	-123.337094	1	2	3	4	0.0582
N	1.386527	1	121.508975	1	158.905755	1	3	2	1	0.6136
O	1.209292	1	117.949276	1	14.796090	1	11	3	2	-0.3295
O	1.208925	1	118.052259	1	-169.032586	1	11	3	2	-0.3270
H	1.115299	1	109.654929	1	-126.683340	1	4	3	2	0.0484
H	1.116830	1	112.520901	1	113.973615	1	4	3	2	0.0356
C	1.544880	1	114.635699	1	-112.411095	1	5	4	3	0.0292
H	1.109887	1	109.332938	1	-60.137369	1	16	5	4	0.0082

121

```
H    1.107860  1  111.523791  1 -178.651481  1  16  5  4      0.0248
H    1.107985  1  112.668589  1   59.851603  1  16  5  4      0.0156
H    1.120553  1  107.261632  1  127.929369  1   5  4  3      0.0565
0    0.000000  0    0.000000  0    0.000000  0   0  0  0
```

PNA.ARC
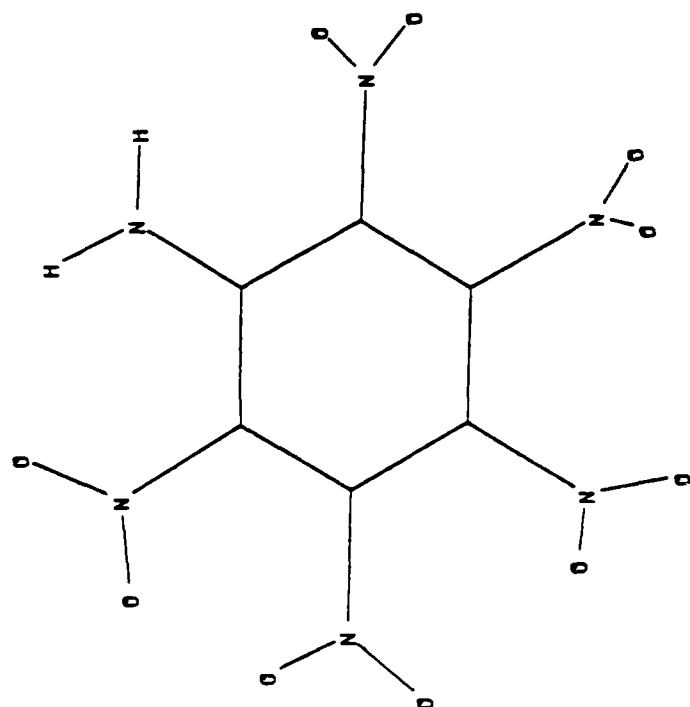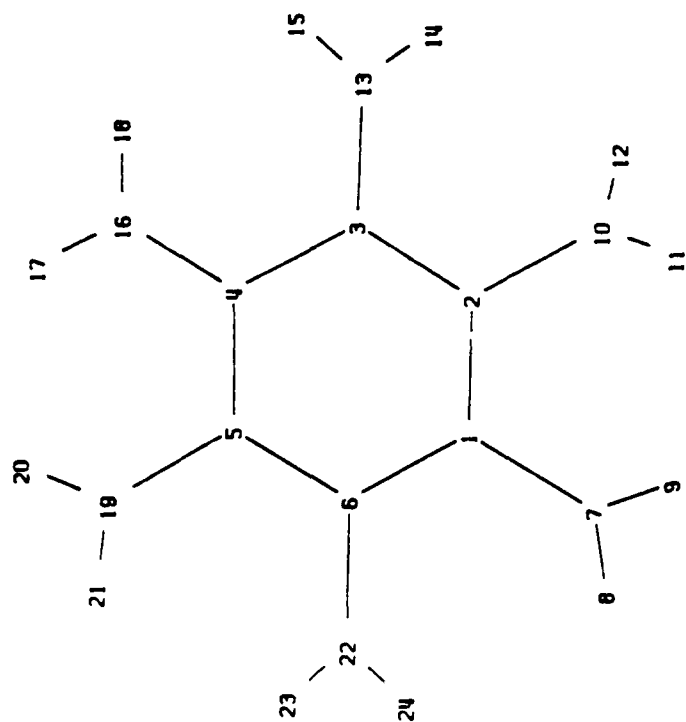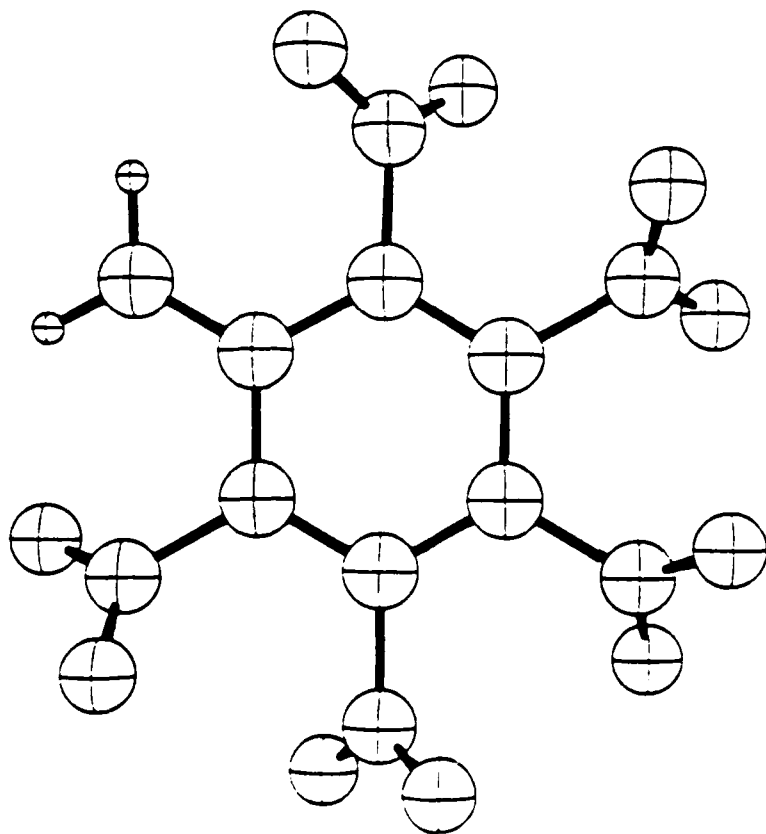
Figure A-7. Pentanitroaniline [Ref. A-6].

123

C6   H2   N6   O10

AM1
RUN ON POTENTIAL RDX/HMX REPLACEMENT pentanitroaniline (PNA)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	82.726640 KCAL
ELECTRONIC ENERGY	=-30880.436105 EV
CORE-CORE REPULSION	= 25656.686415 EV
GRADIENT NORM	= 19567.133028
DIPOLE	=	6.46657 DEBYE
NO. OF FILLED LEVELS	=	58
IONISATION POTENTIAL	=	11.406989 EV
MOLECULAR WEIGHT	=	318.116
SCF CALCULATIONS	=	133
COMPUTATION TIME	= 3861.56 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 AM1
AM1
RUN ON POTENTIAL RDX/HMX REPLACEMENT pentanitroaniline (PNA)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1496
C	1.408455	1	0.000000	0	0.000000	0	1	0	0	0.0526
C	1.399842	1	121.184600	1	0.000000	0	2	1	0	-0.1892
C	1.440749	1	120.460236	1	0.119150	1	3	2	1	0.2569
C	1.442142	1	117.232978	1	-0.096684	1	4	3	2	-0.1906
C	1.401642	1	121.077307	1	-0.470939	1	5	4	3	0.0534
N	1.505815	1	120.234745	1	-179.688953	1	1	2	3	0.5909
O	1.194110	1	117.662390	1	-129.123972	1	7	1	2	-0.2954
O	1.194357	1	117.704103	1	50.971932	1	7	1	2	-0.2959
N	1.518021	1	119.727110	1	-179.378518	1	2	3	4	0.5770
O	1.191940	1	117.513681	1	-125.574757	1	10	2	3	-0.2802
O	1.192754	1	117.226990	1	54.175554	1	10	2	3	-0.2860
N	1.498723	1	119.573426	1	177.360063	1	3	4	5	0.5826
O	1.194562	1	118.270804	1	-130.648161	1	13	3	4	-0.2905
O	1.199692	1	118.156910	1	47.633575	1	13	3	4	-0.3340
N	1.352671	1	121.465739	1	179.946622	1	4	5	6	-0.3237
H	0.997707	1	121.641964	1	-9.667822	1	16	4	5	0.2781
H	0.997666	1	121.493548	1	170.086207	1	16	4	5	0.2768
N	1.499786	1	119.610261	1	-176.922758	1	5	6	1	0.5817
O	1.200201	1	118.366613	1	-136.692830	1	19	5	6	-0.3374
O	1.194874	1	118.314387	1	45.104390	1	19	5	6	-0.2914
N	1.518952	1	119.408020	1	179.051274	1	6	1	2	0.5787
O	1.192711	1	117.336016	1	-125.389566	1	22	6	1	-0.2844

| O | 1.192381 | 1 | 117.367811 | 1 | 54.199998 | 1 | 22 | 6 | 1 | -0.2802 |
| O | 0.000000 | 0 | 0.000000 | 0 | 0.000000 | 0 | 0 | 0 | 0 | |

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C6   H2   N6   O10

MINDO/3
RUN ON POTENTIAL RDX/HMX REPLACEMENT pentanitroaniline (PNA)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-53.697442 KCAL
ELECTRONIC ENERGY	=	-30256.691498 EV
CORE-CORE REPULSION	=	25212.565292 EV
DIPOLE	=	6.02612 DEBYE
NO. OF FILLED LEVELS	=	58
IONISATION POTENTIAL	=	10.460499 EV
MOLECULAR WEIGHT	=	318.116
SCF CALCULATIONS	=	42
COMPUTATION TIME	=	981.55 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 MINDO
MINDO/3
RUN ON POTENTIAL RDX/HMX REPLACEMENT pentanitroaniline (PNA)

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1935
C	1.435239	1	0.000000	0	0.000000	0	1	0	0	0.0286
C	1.425330	1	121.117967	1	0.000000	0	2	1	0	-0.2591
C	1.452964	1	120.137408	1	-1.724633	1	3	2	1	0.3466
C	1.452923	1	118.580356	1	0.345311	1	4	3	2	-0.2595
C	1.425455	1	120.177062	1	1.510881	1	5	4	3	0.0286
N	1.454671	1	120.551881	1	-178.716929	1	1	2	3	1.0948
O	1.220407	1	113.253514	1	-106.841573	1	7	1	2	-0.5221
O	1.220420	1	113.182014	1	73.161099	1	7	1	2	-0.5219
N	1.457282	1	119.300906	1	177.312460	1	2	3	4	1.0620
O	1.221630	1	112.216996	1	-101.738011	1	10	2	3	-0.5143
O	1.220164	1	113.636576	1	77.968977	1	10	2	3	-0.5083
N	1.449857	1	119.300316	1	-179.639710	1	3	4	5	1.1040
O	1.221819	1	113.409680	1	-97.998892	1	13	3	4	-0.5377
O	1.221739	1	113.280020	1	80.023453	1	13	3	4	-0.5329
N	1.335189	1	120.699915	1	-178.438710	1	4	5	6	-0.1426

H	1.013546	1	126.556593	1	3.134124	1	16	4	5	0.1272
H	1.013535	1	126.569664	1	-177.123695	1	16	4	5	0.1272
N	1.449868	1	120.533765	1	177.704572	1	5	6	1	1.1042
O	1.221761	1	113.215253	1	-100.656023	1	19	5	6	-0.5328
O	1.221827	1	113.481114	1	81.308535	1	19	5	6	-0.5383
N	1.457280	1	119.589811	1	-178.469199	1	6	1	2	1.0626
O	1.220200	1	113.582814	1	-103.177531	1	22	6	1	-0.5086
O	1.221564	1	112.256210	1	77.103912	1	22	6	1	-0.5143
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C6   H2   N6   O10

MNDO
RUN ON POTENTIAL RDX/HMX REPLACEMENT pentanitroaniline (PNA)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	145.507404 KCAL
ELECTRONIC ENERGY	=	-30593.663797 EV
CORE-CORE REPULSION	=	25354.777308 EV
GRADIENT NORM	=	5.047533
DIPOLE	=	6.67716 DEBYE
NO. OF FILLED LEVELS	=	58
IONISATION POTENTIAL	=	11.667951 EV
MOLECULAR WEIGHT	=	318.116
SCF CALCULATIONS	=	150
COMPUTATION TIME	=	4195.52 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000
MNDO
RUN ON POTENTIAL RDX/HMX REPLACEMENT pentanitroaniline (PNA)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0775
C	1.412380	1	0.000000	0	0.000000	0	1	0	0	0.1172
C	1.405507	1	120.409747	1	0.000000	0	2	1	0	-0.1227
C	1.440290	1	121.595825	1	-0.988620	1	3	2	1	0.3032
C	1.442203	1	116.768683	1	0.163311	1	4	3	2	-0.1227
C	1.406229	1	120.987468	1	0.597364	1	5	4	3	0.1165
N	1.509287	1	120.388391	1	-179.179473	1	1	2	3	0.4778
O	1.206390	1	118.234853	1	-104.439598	1	7	1	2	-0.2708

O	1.206291	1	118.201510	1	75.568889	1	7	1	2	-0.2690
N	1.516594	1	120.018433	1	178.916839	1	2	3	4	0.4615
O	1.206349	1	117.857073	1	-100.006983	1	10	2	3	-0.2660
O	1.205500	1	118.255386	1	79.558496	1	10	2	3	-0.2570
N	1.508250	1	119.385517	1	-179.737623	1	3	4	5	0.4704
O	1.208234	1	118.322432	1	-91.583586	1	13	3	4	-0.2878
O	1.206764	1	118.559346	1	86.745805	1	13	3	4	-0.2720
N	1.366117	1	121.388673	1	-177.517307	1	4	5	6	-0.2959
H	0.998767	1	122.839825	1	-9.126948	1	16	4	5	0.2233
H	0.998866	1	122.675587	1	-172.412560	1	16	4	5	0.2222
N	1.507230	1	119.130350	1	179.445299	1	5	6	1	0.4729
O	1.207951	1	118.432980	1	-99.241891	1	19	5	6	-0.2845
O	1.207058	1	118.469271	1	81.579841	1	19	5	6	-0.2767
N	1.519218	1	119.412972	1	179.492405	1	6	1	2	0.4613
O	1.205503	1	118.229271	1	-101.032897	1	22	6	1	-0.2603
O	1.205932	1	117.900293	1	79.040023	1	22	6	1	-0.2635
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	
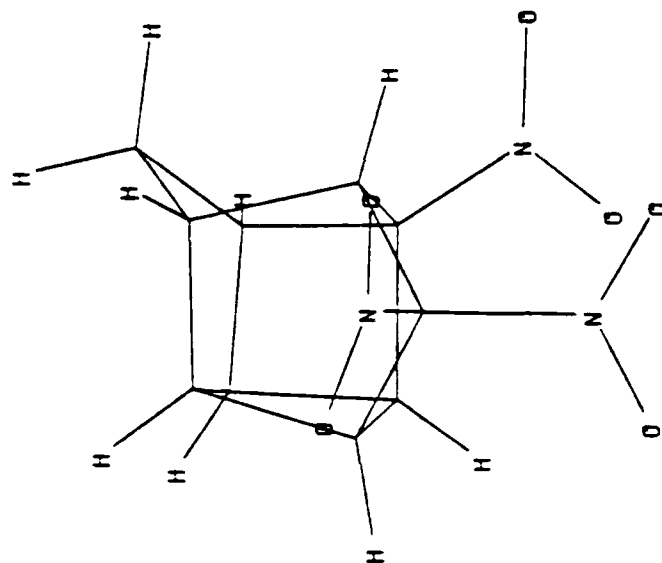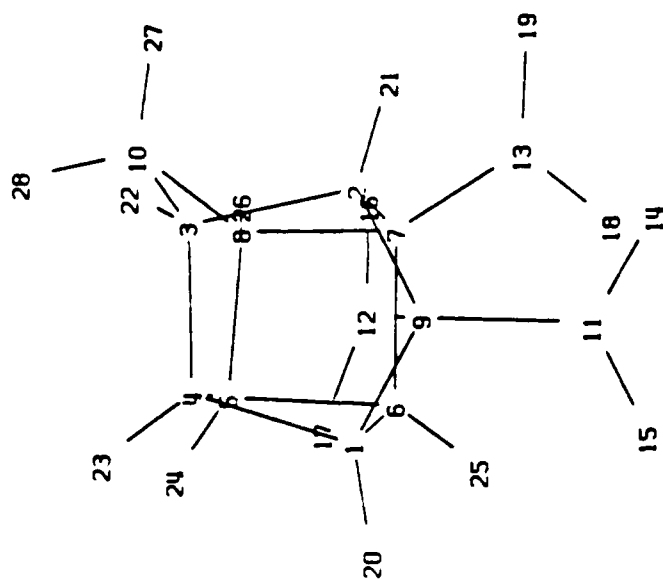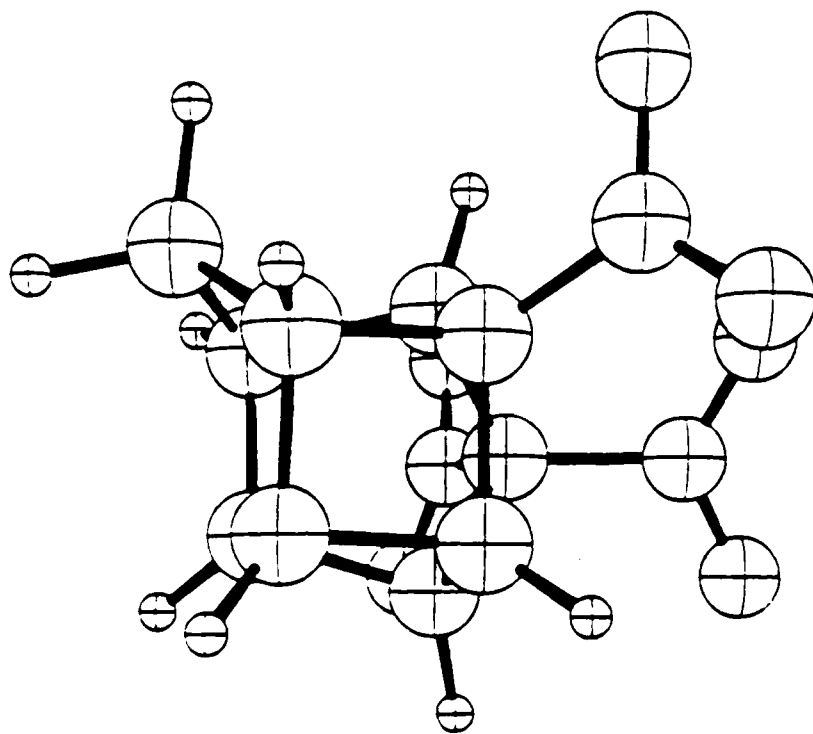
TRINPCO.ARC

Figure A 8. 6,6,8-Trinitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]-
decane [Ref. A-7].

VERSION   3.00

C10 H9 N3   O6   17-JAN-86

Run on 6,6,8-trinitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TRINPCD)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	87.781465 KCAL
ELECTRONIC ENERGY	=-24987.481472 EV
CORE-CORE REPULSION	= 21052.108380 EV
DIPOLE	=	7.41250 DEBYE
NO. OF FILLED LEVELS	=	50
IONISATION POTENTIAL	=	11.892997 EV
MOLECULAR WEIGHT	=	267.198
SCF CALCULATIONS	=	139
COMPUTATION TIME	= 86553.52 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 RESTART
Run on 6,6,8-trinitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TRINPCD)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1120
C	2.324531	1	0.000000	0	0.000000	0	1	0	0	-0.0808
C	1.567647	1	77.058054	1	0.000000	0	2	1	0	-0.1187
C	1.563706	1	100.907137	1	12.042458	1	3	2	1	-0.1165
C	1.579142	1	102.890341	1	75.089723	1	4	3	2	-0.1224
C	1.554157	1	76.822222	1	-104.285604	1	1	2	3	-0.1083
C	1.586525	1	103.555416	1	0.496709	1	6	1	2	-0.1070
C	1.597110	1	89.851442	1	104.120051	1	7	6	1	-0.0803
C	1.560752	1	101.973297	1	45.365011	1	2	3	4	-0.0688
C	1.535903	1	102.220513	1	119.749366	1	3	2	1	-0.1549
N	1.551917	1	113.566153	1	-172.391370	1	9	2	3	0.5317
N	1.551640	1	112.347988	1	64.108026	1	9	2	3	0.5333
N	1.494569	1	119.449337	1	-133.333125	1	7	6	1	0.5547
O	1.192923	1	117.864455	1	-17.989732	1	11	9	2	-0.3046
O	1.193832	1	117.514869	1	162.348716	1	11	9	2	-0.3092
O	1.194549	1	117.620823	1	46.918597	1	12	9	2	-0.3168
O	1.193282	1	117.990003	1	-132.760439	1	12	9	2	-0.3077
O	1.199860	1	118.496578	1	-7.373773	1	13	7	6	-0.3431
O	1.199247	1	118.586809	1	174.174195	1	13	7	6	-0.3368
H	1.102441	1	158.339998	1	115.777627	1	1	2	3	0.1765
H	1.107751	1	116.835691	1	173.152974	1	2	3	4	0.1852
H	1.105381	1	115.142244	1	-113.508303	1	3	2	1	0.1443
H	1.098026	1	116.963902	1	-151.931867	1	4	3	2	0.1479
H	1.092423	1	120.474726	1	140.145395	1	5	4	3	0.1517

H	1.094946	1	122.337441	1	-138.609497	1	6	1	2	0.1746
H	1.100406	1	117.467375	1	107.216618	1	8	7	6	0.1511
H	1.114989	1	112.291020	1	62.641809	1	10	3	2	0.1207
H	1.114751	1	112.455370	1	-173.411859	1	10	3	2	0.1162
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C10 H9 N3 O6

Run on 6,6,8-trinitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane (TRINPCD)

12-JAN-86

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	73.990430 KCAL
ELECTRONIC ENERGY	=-24362.358957 EV
CORE-CORE REPULSION	= 20528.738972 EV
DIPOLE	=	6.67778 DEBYE
NO. OF FILLED LEVELS	=	50
IONISATION POTENTIAL	=	10.429627 EV
MOLECULAR WEIGHT	=	267.198
SCF CALCULATIONS	=	123
COMPUTATION TIME	= 47287.66 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000 RESTART
Run on 6,6,8-trinitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TRINPCD)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0676
C	2.281026	1	0.000000	0	0.000000	0	1	0	0	0.1045
C	1.585763	1	78.902141	1	0.000000	0	2	1	0	0.0164
C	1.583522	1	98.532456	1	10.980615	1	3	2	1	0.0202
C	1.577980	1	102.121070	1	77.461702	1	4	3	2	0.0100
C	1.562735	1	77.574792	1	-101.723684	1	1	2	3	0.0375
C	1.601811	1	104.474812	1	-0.166314	1	6	1	2	-0.1759
C	1.614494	1	89.153397	1	103.552576	1	7	6	1	0.0662
C	1.600285	1	105.735937	1	46.268346	1	2	3	4	-0.3320
C	1.541585	1	105.011506	1	120.160405	1	3	2	1	0.0414
N	1.489876	1	118.006544	1	-171.988027	1	9	2	3	1.0997
N	1.490922	1	113.281480	1	65.397965	1	9	2	3	1.1006
N	1.457782	1	123.038017	1	-135.659708	1	7	6	1	1.1019

O	1.219684	1	115.134941	1	-16.173503	1	11	9	2	-0.5306
O	1.222938	1	113.186142	1	163.389525	1	11	9	2	-0.5427
O	1.222672	1	113.713977	1	64.388183	1	12	9	2	-0.5426
O	1.221040	1	114.916053	1	-114.910035	1	12	9	2	-0.5338
O	1.224394	1	114.407131	1	-4.920353	1	13	7	6	-0.5609
O	1.225158	1	113.814908	1	178.583774	1	13	7	6	-0.5612
H	1.112164	1	162.283726	1	118.646448	1	1	2	3	0.0269
H	1.114291	1	112.840707	1	173.118431	1	2	3	4	0.0261
H	1.112318	1	115.723304	1	-113.115461	1	3	2	1	0.0032
H	1.109218	1	116.801771	1	-150.825985	1	4	3	2	0.0144
H	1.106950	1	120.340011	1	139.133649	1	5	4	3	0.0126
H	1.108153	1	119.689849	1	-141.350072	1	6	1	2	0.0264
H	1.111019	1	117.708039	1	107.479585	1	8	7	6	0.0048
H	1.111821	1	114.842561	1	66.773446	1	10	3	2	0.0044
H	1.113833	1	113.858250	1	-173.869215	1	10	3	2	-0.0053
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF   MNDO   CALCULATION

VERSION   3.00

C10 H9   N3   O6

Run on 6,6,8-trinitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TRINPCD)

4-JAN-86

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	109.177445 KCAL
ELECTRONIC ENERGY	=-24746.325647 EV
CORE-CORE REPULSION	= 20799.309303 EV
GRADIENT NORM	=	3.545379
DIPOLE	=	7.70888 DEBYE
NO. OF FILLED LEVELS	=	50
IONISATION POTENTIAL	=	11.861376 EV
MOLECULAR WEIGHT	=	267.198
SCF CALCULATIONS	=	180
COMPUTATION TIME	= 61711.10 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 RESTART
Run on 6,6,8-trinitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TRINPCD)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0419

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C	2.315095	1	0.000000	0	0.000000	0	1	0	0	-0.0045
C	1.587786	1	77.776277	1	0.000000	0	2	1	0	-0.0596
C	1.581014	1	99.834688	1	11.520974	1	3	2	1	-0.0483
C	1.579451	1	102.541815	1	76.226366	1	4	3	2	-0.0622
C	1.566249	1	77.116136	1	-102.791774	1	1	2	3	-0.0377
C	1.587488	1	103.679617	1	0.736611	1	6	1	2	-0.0508
C	1.594657	1	90.066388	1	104.398108	1	7	6	1	-0.0219
C	1.574638	1	103.320743	1	45.291186	1	2	3	4	0.0578
C	1.551892	1	103.836811	1	120.072517	1	3	2	1	0.0033
N	1.559745	1	116.378371	1	-174.663518	1	9	2	3	0.4316
N	1.560859	1	114.135729	1	66.982917	1	9	2	3	0.4318
N	1.519189	1	120.774296	1	-133.388493	1	7	6	1	0.4670
O	1.205379	1	119.234808	1	-25.748246	1	11	9	2	-0.2796
O	1.207026	1	118.329860	1	155.567249	1	11	9	2	-0.2914
O	1.207258	1	118.511724	1	52.399278	1	12	9	2	-0.2927
O	1.206211	1	119.402290	1	-128.148936	1	12	9	2	-0.2895
O	1.208386	1	119.593619	1	8.015041	1	13	7	6	-0.3151
O	1.209347	1	118.693088	1	-170.542045	1	13	7	6	-0.3182
H	1.097927	1	160.601889	1	117.502780	1	1	2	3	0.1048
H	1.101249	1	114.863788	1	173.275145	1	2	3	4	0.1079
H	1.099615	1	115.798602	1	-113.414464	1	3	2	1	0.0718
H	1.093806	1	116.817550	1	-151.063748	1	4	3	2	0.0814
H	1.089786	1	120.528340	1	139.532705	1	5	4	3	0.0855
H	1.090956	1	120.597555	1	-140.281819	1	6	1	2	0.1056
H	1.096256	1	118.380717	1	106.833790	1	8	7	6	0.0815
H	1.106650	1	113.719822	1	63.981051	1	10	3	2	0.0446
H	1.107365	1	113.310535	1	-173.733488	1	10	3	2	0.0386
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

BFONEN.ARC
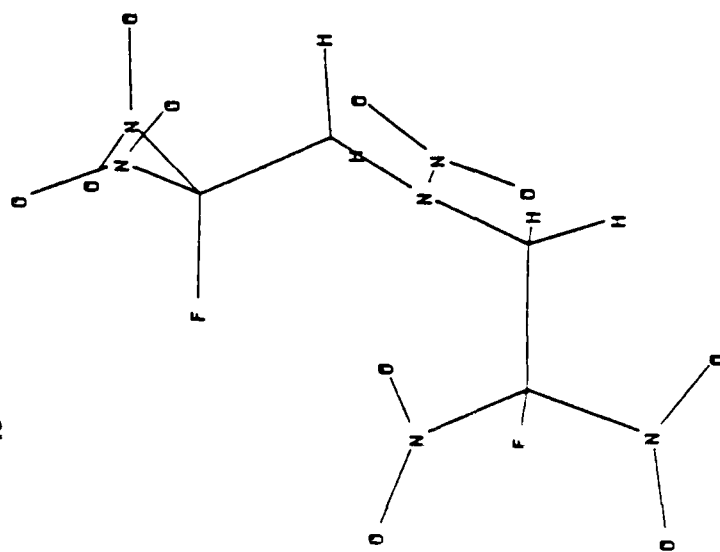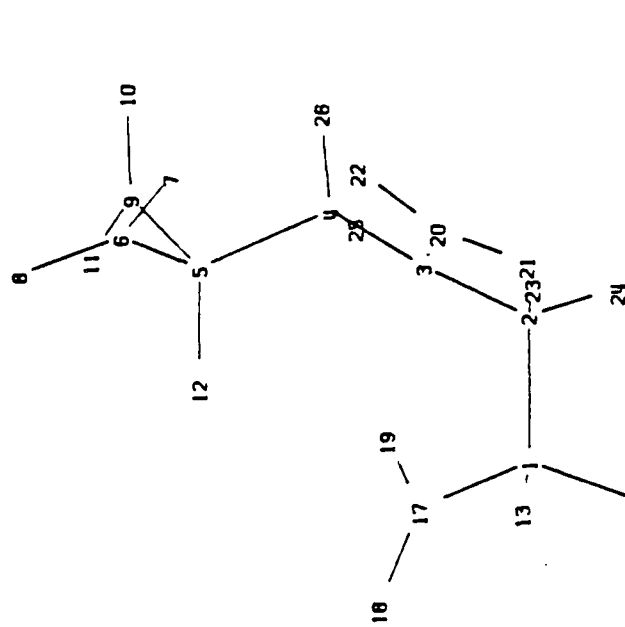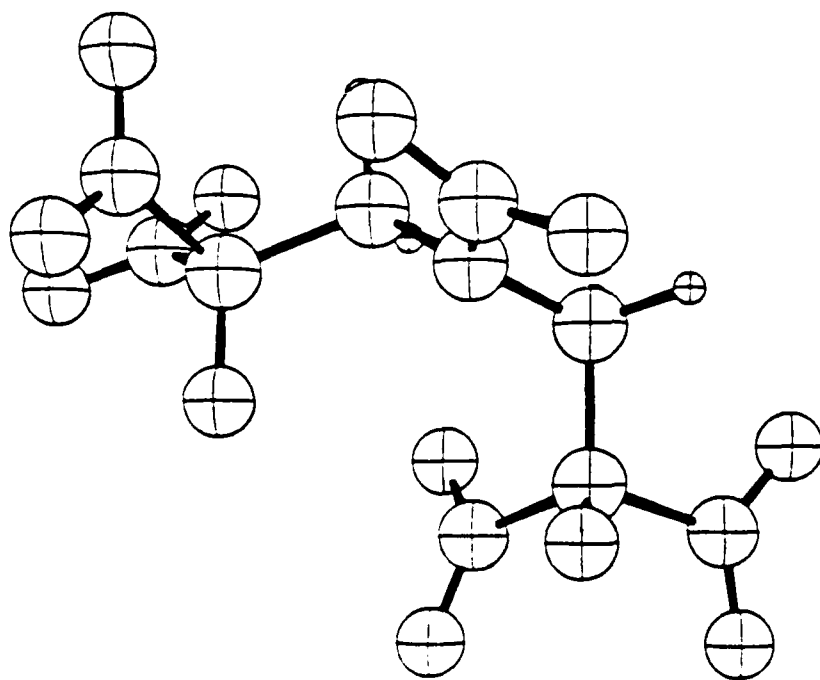
Figure A-9. Bis(2-fluoro-2,2-dinitroethyl)nitramine [Ref. A-8].

VERSION 3.00

C4 H4 N6 O10 F2

27-JAN-86

AM1
Bis(2-fluoro-2,2-dinitroethyl)nitramine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-53.930705 KCAL
ELECTRONIC ENERGY	=	-35304.000864 EV
CORE-CORE REPULSION	=	29348.460244 EV
DIPOLE	=	4.31870 DEBYE
NO. OF FILLED LEVELS	=	62
IONISATION POTENTIAL	=	12.304493 EV
MOLECULAR WEIGHT	=	334.107
SCF CALCULATIONS	=	80
COMPUTATION TIME	=	218131.26 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 RESTART
MINDO/3
Bis(2-fluoro-2,2-dinitroethyl)nitramine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.1439
C	1.590491	1	0.000000	0	0.000000	0	1	0	0	-0.0444
N	1.448222	1	111.988165	1	0.000000	0	2	1	0	-0.3581
C	1.450419	1	117.836364	1	-107.605658	1	3	2	1	-0.0534
C	1.591280	1	113.825165	1	123.766405	1	4	3	2	0.1279
N	1.634205	1	107.219934	1	-157.925712	1	5	4	3	0.5031
O	1.188676	1	116.146637	1	-2.048934	1	6	5	4	-0.3065
O	1.184621	1	117.078188	1	179.105062	1	6	5	4	-0.2694
N	1.621416	1	109.221013	1	88.778358	1	5	4	3	0.5096
O	1.189729	1	115.207634	1	52.862064	1	9	5	4	-0.3061
O	1.183480	1	117.756258	1	-126.743369	1	9	5	4	-0.2593
F	1.302944	1	114.607634	1	-36.022624	1	5	4	3	-0.1234
F	1.300870	1	114.303988	1	-56.408632	1	1	2	3	-0.1103
N	1.630364	1	107.121160	1	-178.704585	1	1	2	3	0.4941
O	1.189929	1	115.534920	1	0.476221	1	14	1	2	-0.3112
O	1.183987	1	117.722797	1	-178.593226	1	14	1	2	-0.2600
N	1.616708	1	108.590222	1	67.906418	1	1	2	3	0.4935
O	1.182144	1	118.777378	1	-156.854279	1	17	1	2	-0.2379
O	1.195344	1	114.951998	1	23.937481	1	17	1	2	-0.3545
N	1.414920	1	117.761234	1	98.051601	1	3	2	1	0.6416
O	1.196206	1	117.261286	1	-13.951392	1	20	3	2	-0.3055
O	1.195955	1	117.336866	1	167.430855	1	20	3	2	-0.3137
H	1.128125	1	110.722009	1	12.402751	1	2	3	4	0.1694

H	1.133093	1	111.843034	1	133.614479	1	2	3	4	0.1778
H	1.132683	1	108.076765	1	5.498265	1	4	3	2	0.1822
H	1.130774	1	112.259699	1	-114.647633	1	4	3	2	0.1708
0	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C4   H4   N6   O10 F2

18-JAN-86

MINDO/3
Bis(2-fluoro-2,2-dinitroethyl)nitramine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED


```
HEAT OF FORMATION       =  -169.714151 KCAL
ELECTRONIC ENERGY       =-34886.496715 EV
CORE-CORE REPULSION     = 29109.936054 EV
DIPOLE                  =       0.15500 DEBYE
NO. OF FILLED LEVELS    =      62
IONISATION POTENTIAL    =      11.157086 EV
MOLECULAR WEIGHT        =     334.107
SCF CALCULATIONS        =     226
COMPUTATION TIME        =161886.70 SECONDS
```


FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000 RESTART
MINDO/3
Bis(2-fluoro-2,2-dinitroethyl)nitramine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1882
C	1.530140	1	0.000000	0	0.000000	0	1	0	0	0.2518
N	1.487352	1	116.436650	1	0.000000	0	2	1	0	-0.2549
C	1.483313	1	114.324144	1	-114.110361	1	3	2	1	0.2605
C	1.530252	1	118.501152	1	-120.516153	1	4	3	2	-0.1985
N	1.476692	1	115.626670	1	-158.819198	1	5	4	3	1.0943
0	1.224116	1	111.520087	1	-81.649995	1	6	5	4	-0.5475
0	1.214901	1	115.006197	1	96.719602	1	6	5	4	-0.4873
N	1.467029	1	122.397460	1	56.266377	1	5	4	3	1.0983
0	1.224451	1	113.922654	1	10.893344	1	9	5	4	-0.5612
0	1.219740	1	113.922733	1	-167.125319	1	9	5	4	-0.5169
F	1.402813	1	78.031769	1	-44.664582	1	5	4	3	-0.1360
F	1.402656	1	77.405645	1	-45.251885	1	1	2	3	-0.1494
N	1.478632	1	120.972517	1	-149.135079	1	1	2	3	1.1033

										CHARGE
O	1.219811	1	114.367922	1	-31.097039	1	14	1	2	-0.5271
O	1.218689	1	112.571166	1	148.605075	1	14	1	2	-0.5114
N	1.467740	1	117.709477	1	66.145265	1	1	2	3	1.0796
O	1.220249	1	114.494976	1	-86.026543	1	17	1	2	-0.5195
O	1.223714	1	112.909865	1	91.493063	1	17	1	2	-0.5408
N	1.311712	1	122.374100	1	64.885043	1	3	2	1	1.0867
O	1.246445	1	117.710435	1	-8.365149	1	20	3	2	-0.4088
O	1.247644	1	117.898241	1	170.741646	1	20	3	2	-0.4051
H	1.128361	1	106.936139	1	11.435164	1	2	3	4	-0.0097
H	1.125010	1	109.180155	1	120.187478	1	2	3	4	0.0167
H	1.127359	1	109.015925	1	114.513286	1	4	3	2	-0.0072
H	1.129715	1	106.848289	1	6.925950	1	4	3	2	-0.0217
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C4 H4 N6 O10 F2

5-JAN-86

MNDO
Bis(2-fluoro-2,2-dinitroethyl)nitramine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   31.217111 KCAL
ELECTRONIC ENERGY   =-34780.584634 EV
CORE-CORE REPULSION   = 28809.227048 EV
DIPOLE   =   4.93442 DEBYE
NO. OF FILLED LEVELS   =   62
IONISATION POTENTIAL   =   12.786974 EV
MOLECULAR WEIGHT   =   334.107
SCF CALCULATIONS   =   71
COMPUTATION TIME   = 77807.27 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 RESTART
MNDO
Bis(2-fluoro-2,2-dinitroethyl)nitramine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.2595
C	1.588624	1	0.000000	0	0.000000	0	1	0	0	0.1385
N	1.484635	1	109.812269	1	0.000000	0	2	1	0	-0.3888
C	1.483907	1	116.588273	1	-138.849050	1	3	2	1	0.1404
C	1.589908	1	110.477935	1	132.493765	1	4	3	2	0.2655

N	1.600443	1	108.862048	1	-159.607223	1	5	4	3	0.3926
O	1.205729	1	117.586749	1	-71.633669	1	6	5	4	-0.2903
O	1.201282	1	118.917393	1	106.608639	1	6	5	4	-0.2456
N	1.598365	1	115.267139	1	84.672934	1	5	4	3	0.4111
O	1.204105	1	118.433394	1	9.254187	1	9	5	4	-0.2901
O	1.201111	1	117.938051	1	-171.585099	1	9	5	4	-0.2426
F	1.323079	1	114.459651	1	-39.085999	1	5	4	3	-0.1301
F	1.326262	1	113.689852	1	-66.401139	1	1	2	3	-0.1440
N	1.603375	1	112.534776	1	174.110467	1	1	2	3	0.4056
O	1.204276	1	118.697969	1	7.190522	1	14	1	2	-0.2909
O	1.201461	1	117.862683	1	-173.864985	1	14	1	2	-0.2484
N	1.591170	1	111.939527	1	57.242932	1	1	2	3	0.4142
O	1.199176	1	119.405113	1	-121.512601	1	17	1	2	-0.2255
O	1.206983	1	116.726287	1	58.220649	1	17	1	2	-0.3037
N	1.448515	1	114.992244	1	82.493193	1	3	2	1	0.5521
O	1.204024	1	119.036531	1	60.282248	1	20	3	2	-0.2870
O	1.197485	1	114.887240	1	-118.849009	1	20	3	2	-0.2175
H	1.116134	1	109.750054	1	-18.910997	1	2	3	4	0.0838
H	1.118667	1	112.993761	1	99.639023	1	2	3	4	0.0824
H	1.118299	1	109.245631	1	14.872513	1	4	3	2	0.0689
H	1.116832	1	113.256803	1	-102.686567	1	4	3	2	0.0898
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	
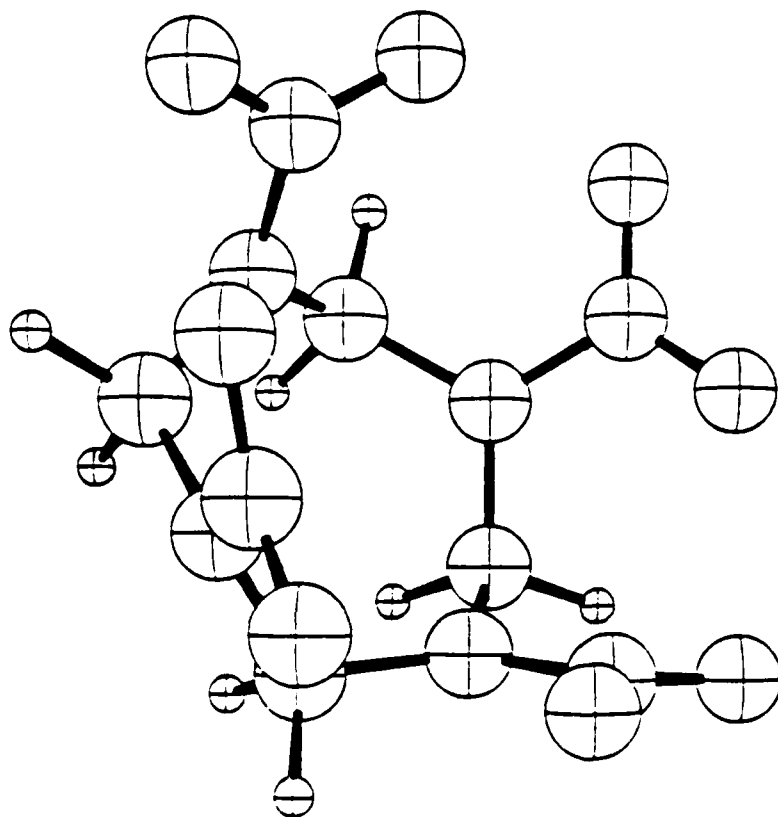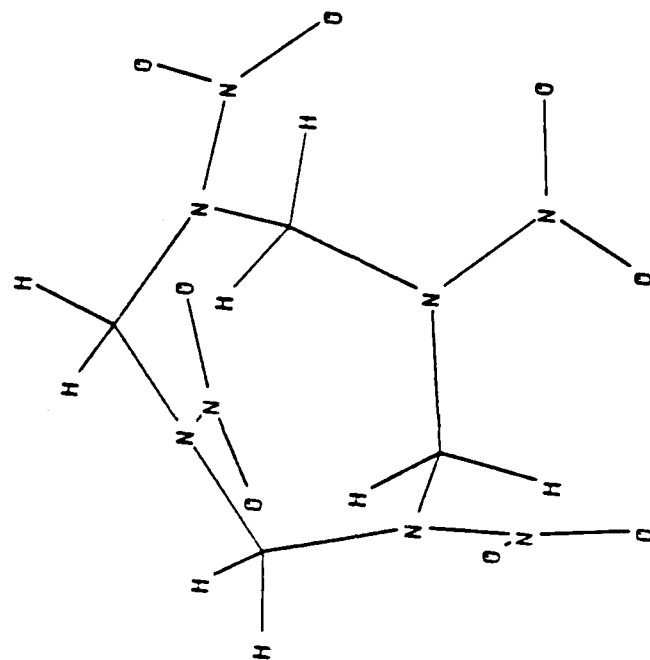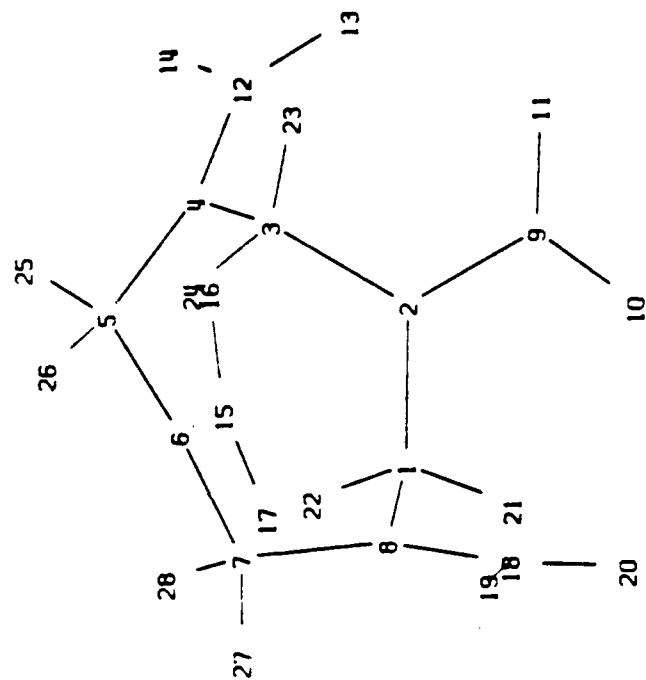
Figure A-10. 1,3,5,7-Tetranitro-1,3,5,7-tetraazacyclooctane
[Ref. A-9].

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SUMMARY OF AM1 CALCULATION

VERSION 3.00

C4 H8 N8 O8

5-MAR-86

AM1
RUN ON 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	144.396911 KCAL
ELECTRONIC ENERGY	=	-30574.853753 EV
CORE-CORE REPULSION	=	25751.044935 EV
DIPOLE	=	10.81968 DEBYE
NO. OF FILLED LEVELS	=	56
IONISATION POTENTIAL	=	11.779905 EV
MOLECULAR WEIGHT	=	296.156
SCF CALCULATIONS	=	86
COMPUTATION TIME	=	118043.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS T=36000 AM1 PULAY PRECISE RESTART
AM1
RUN ON 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX)

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0840
N	1.461484	1	0.000000	0	0.000000	0	1	0	0	-0.4009
C	1.459213	1	119.533526	1	0.000000	0	2	1	0	0.0845
N	1.461256	1	118.949504	1	83.352377	1	3	2	1	-0.3986
C	1.459472	1	119.427810	1	-80.706742	1	4	3	2	0.0854
N	1.461645	1	118.693259	1	80.001066	1	5	4	3	-0.4034
C	1.458958	1	119.495798	1	-83.020576	1	6	5	4	0.0851
N	1.461349	1	118.918057	1	83.880271	1	7	6	5	-0.3977
N	1.409358	1	119.148926	1	79.257141	1	2	1	8	0.6338
O	1.198975	1	117.460263	1	-6.215426	1	9	2	1	-0.3285
O	1.195461	1	117.374877	1	-27.348517	1	9	2	3	-0.2936
N	1.410548	1	119.156214	1	80.655392	1	4	3	2	0.6340
O	1.198556	1	117.501972	1	-5.322272	1	12	4	3	-0.3248
O	1.195753	1	117.328911	1	-27.316753	1	12	4	5	-0.2966
N	1.408258	1	119.229495	1	79.827152	1	6	5	4	0.6347
O	1.199098	1	117.400271	1	-5.810781	1	15	6	5	-0.3288
O	1.195457	1	117.435247	1	-26.059219	1	15	6	7	-0.2937
N	1.410480	1	119.210211	1	80.583190	1	8	7	6	0.6344
O	1.198464	1	117.497664	1	-4.761885	1	18	8	7	-0.3240
O	1.195754	1	117.272839	1	-26.952170	1	18	8	1	-0.2968
H	1.138442	1	107.874833	1	-157.127752	1	1	8	7	0.1743
H	1.131362	1	106.427876	1	-39.900739	1	1	8	7	0.1287
H	1.138446	1	107.733472	1	-153.681225	1	3	2	1	0.1739
H	1.131447	1	106.577770	1	-36.405298	1	3	2	1	0.1288

H	1.138280	1·	107.922679	1	-157.007087	1	5	4	3	0.1747
H	1.131444	1	106.514840	1	-39.689953	1	5	4	3	0.1287
H	1.138430	1	107.738430	1	-153.203362	1	7	6	5	0.1736
H	1.131458	1	106.595709	1	-35.891921	1	7	6	5	0.1287
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C4 H8 N8 O8

21-FEB-86

MINDO/3
RUN ON 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-29.132261 KCAL
ELECTRONIC ENERGY	=-29509.839961 EV
CORE-CORE REPULSION	= 24866.439050 EV
DIPOLE	= 9.32803 DEBYE
NO. OF FILLED LEVELS	= 56
IONISATION POTENTIAL	= 10.598886 EV
MOLECULAR WEIGHT	= 296.156
SCF CALCULATIONS	= 9
COMPUTATION TIME	= 2643.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
    BONDS T=36000 MINDO3 PULAY PRECISE
    MINDO/3
    RUN ON 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3220
N	1.453664	1	0.000000	0	0.000000	0	1	0	0	-0.3759
C	1.451154	1	117.579945	1	0.000000	0	2	1	0	0.3223
N	1.455465	1	111.530578	1	90.401807	1	3	2	1	-0.3724
C	1.452848	1	117.092087	1	-89.728324	1	4	3	2	0.3222
N	1.453317	1	111.689998	1	89.844659	1	5	4	3	-0.3764
C	1.450902	1	117.444724	1	-90.589146	1	6	5	4	0.3226
N	1.455223	1	111.698356	1	90.479102	1	7	6	5	-0.3720
N	1.344711	1	120.090171	1	97.938744	1	2	1	8	1.2072
O	1.222141	1	113.481730	1	-46.552877	1	9	2	1	-0.5566
O	1.221415	1	114.775162	1	-39.484341	1	9	2	3	-0.5489
N	1.341874	1	120.306976	1	98.803027	1	4	3	2	1.2061
O	1.222892	1	113.517911	1	-42.247511	1	12	4	3	-0.5599

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O	1.221985	1	114.919495	1	-35.071144	1	12	4	5	-0.5517
N	1.344729	1	120.215744	1	97.632806	1	6	5	4	1.2077
O	1.221976	1	113.510709	1	-46.905801	1	15	6	5	-0.5563
O	1.221376	1	114.727111	1	-40.007284	1	15	6	7	-0.5487
N	1.341798	1	120.345067	1	98.777630	1	8	7	6	1.2061
O	1.222885	1	113.525813	1	-42.113897	1	18	8	7	-0.5601
O	1.221922	1	114.919491	1	-35.099824	1	18	8	1	-0.5515
H	1.130867	1	114.560338	1	-142.050558	1	1	8	7	-0.0035
H	1.137644	1	110.006473	1	-32.027324	1	1	8	7	-0.0433
H	1.130794	1	114.500996	1	-141.142543	1	3	2	1	-0.0027
H	1.137497	1	110.174792	1	-31.028626	1	3	2	1	-0.0433
H	1.130979	1	114.488967	1	-141.859960	1	5	4	3	-0.0039
H	1.137408	1	110.069665	1	-31.757864	1	5	4	3	-0.0427
H	1.130941	1	114.469824	1	-141.049164	1	7	6	5	-0.0031
H	1.137558	1	110.095573	1	-31.011037	1	7	6	5	-0.0433
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C4 H8 N8 O8

1-MAR-86

MNDO
RUN ON 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	149.185456 KCAL
ELECTRONIC ENERGY	=	-30092.095595 EV
CORE-CORE REPULSION	=	25250.136832 EV
DIPOLE	=	10.49568 DEBYE
NO. OF FILLED LEVELS	=	56
IONISATION POTENTIAL	=	12.138200 EV
MOLECULAR WEIGHT	=	296.156
SCF CALCULATIONS	=	85
COMPUTATION TIME	=	80573.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS T=36000 PULAY PRECISE RESTART
MNDO
RUN ON 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3614
N	1.478457	1	0.000000	0	0.000000	0	1	0	0	-0.4890

C	1.475677	1	121.484703	1.	0.000000	0	2	1	0	0.3627
N	1.479208	1	112.513557	1	86.643937	1	3	2	1	-0.4875
C	1.475629	1	121.306881	1	-86.270119	1	4	3	2	0.3623
N	1.478754	1	112.369454	1	85.843241	1	5	4	3	-0.4890
C	1.475545	1	121.316964	1	-86.500375	1	6	5	4	0.3619
N	1.479308	1	112.772279	1	86.882574	1	7	6	5	-0.4854
N	1.410576	1	118.948287	1	91.713883	1	2	1	8	0.6115
O	1.204330	1	117.951373	1	-41.601449	1	9	2	1	-0.2955
O	1.205203	1	117.384874	1	-46.166792	1	9	2	3	-0.2966
N	1.409530	1	119.040395	1	91.385847	1	4	3	2	0.6124
O	1.204424	1	117.987844	1	-39.564007	1	12	4	3	-0.2975
O	1.205149	1	117.419270	1	-44.366863	1	12	4	5	-0.2980
N	1.410140	1	119.026653	1	91.204570	1	6	5	4	0.6123
O	1.204266	1	117.968272	1	-41.003198	1	15	6	5	-0.2963
O	1.205003	1	117.384023	1	-45.780866	1	15	6	7	-0.2964
N	1.409770	1	119.093174	1	90.434443	1	8	7	6	0.6114
O	1.204464	1	118.078176	1	-38.618920	1	18	8	7	-0.2985
O	1.205153	1	117.349340	1	-45.123714	1	18	8	1	-0.2972
H	1.120186	1	111.793123	1	-150.105516	1	1	8	7	0.0737
H	1.123409	1	107.978647	1	-34.157384	1	1	8	7	0.0343
H	1.120110	1	111.896084	1	-148.573122	1	3	2	1	0.0734
H	1.122901	1	108.125909	1	-32.402171	1	3	2	1	0.0341
H	1.120077	1	111.984716	1	-149.425087	1	5	4	3	0.0736
H	1.122915	1	108.144324	1	-33.209514	1	5	4	3	0.0342
H	1.120210	1	111.877639	1	-148.302549	1	7	6	5	0.0735
H	1.122941	1	108.130927	1	-32.166433	1	7	6	5	0.0343
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

ONDO.ARC
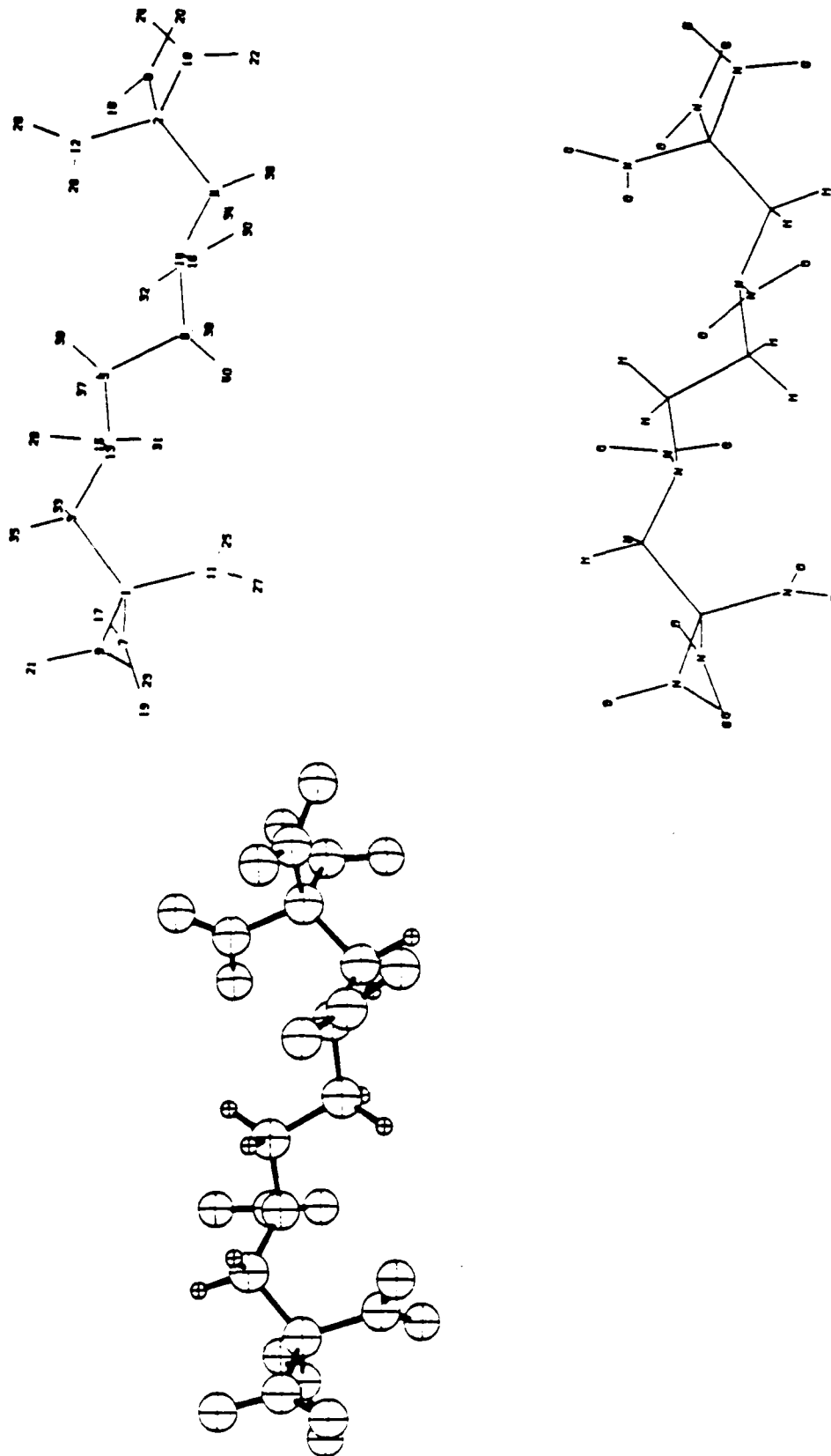
Figure A-11. 1,1,1,3,6,8,8,8-Octanitro-3,6-diazaoctane
[Ref. A-10].

143

C6   H8   N10 O16

25-MAY-86

RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,1,1,3,6,8,8,8-octanitro-
3,6-diazaoctane (ONDO)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	128.977894 KCAL
ELECTRONIC ENERGY	=-59765.271106 EV
CORE-CORE REPULSION	= 51720.268270 EV
DIPOLE	=	0.11986 DEBYE
NO. OF FILLED LEVELS	=	89
IONISATION POTENTIAL	=	11.934799 EV
MOLECULAR WEIGHT	=	476.187
SCF CALCULATIONS	=	11
COMPUTATION TIME	=843548.20 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 RESTART
RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,1,1,3,6,8,8,8-octanitro-
3,6-diazaoctane (ONDO)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1463
C	7.760773	1	0.000000	0	0.000000	0	1	0	0	-0.1458
C	6.821059	1	9.977329	1	0.000000	0	2	1	0	-0.0324
C	6.106337	1	12.494376	1	1.462324	1	3	2	1	-0.0350
C	3.703162	1	7.837163	1	18.642102	1	4	3	2	-0.0452
C	1.550778	1	30.150557	1	-1.942424	1	5	4	3	-0.0472
N	1.580352	1	103.210393	1	104.525634	1	1	2	3	0.5580
N	1.580186	1	100.928513	1	-106.325886	1	2	3	4	0.5580
N	1.584399	1	145.039257	1	-59.149573	1	1	2	3	0.5449
N	1.584404	1	148.659047	1	70.734679	1	2	3	4	0.5451
N	1.578437	1	67.721972	1	-148.334291	1	1	2	3	0.5376
N	1.578857	1	60.615755	1	145.934686	1	2	3	4	0.5385
N	1.447205	1	28.128749	1	-76.439396	1	3	2	1	-0.3469
N	1.466934	1	111.769549	1	28.713584	1	6	5	4	-0.3436
N	1.409918	1	117.984118	1	-146.829332	1	13	3	2	0.6337
N	1.410914	1	118.043510	1	73.944419	1	14	6	5	0.6327
O	1.188928	1	116.409574	1	31.050757	1	7	1	2	-0.2829
O	1.188852	1	116.421720	1	-22.466881	1	8	2	3	-0.2819
O	1.187572	1	117.306913	1	-146.755269	1	7	1	2	-0.2718
O	1.187706	1	117.315821	1	155.374861	1	8	2	3	-0.2728
O	1.189759	1	116.158001	1	44.043872	1	9	1	2	-0.2934
O	1.189714	1	116.169770	1	-58.650140	1	10	2	3	-0.2933
O	1.186020	1	117.297631	1	-135.459877	1	9	1	2	-0.2588
O	1.186085	1	117.285138	1	120.870361	1	10	2	3	-0.2597

O	1.192434	1	115.550447	1	53.756226	1	11	1	2	-0.3057
O	1.192450	1	115.408476	1	-60.640653	1	12	2	3	-0.3057
O	1.186285	1	118.558931	1	-127.179754	1	11	1	2	-0.2578
O	1.186078	1	118.641835	1	120.286039	1	12	2	3	-0.2571
O	1.200518	1	117.509538	1	-11.532127	1	15	13	3	-0.3426
O	1.200601	1	117.467721	1	161.874310	1	16	14	6	-0.3425
O	1.196360	1	117.569567	1	170.995428	1	15	13	3	-0.3066
O	1.196378	1	117.673342	1	-20.737543	1	16	14	6	-0.3071
H	1.130280	1	82.132482	1	105.489945	1	3	2	1	0.1707
H	1.130397	1	85.220738	1	-106.703521	1	4	3	2	0.1704
H	1.133531	1	125.161844	1	-147.821749	1	3	2	1	0.1737
H	1.133596	1	134.083825	1	142.648937	1	4	3	2	0.1743
H	1.129344	1	106.208809	1	97.985512	1	5	4	3	0.1538
H	1.129615	1	108.769482	1	-89.892901	1	6	5	4	0.1538
H	1.128262	1	82.401123	1	-154.074401	1	5	4	3	0.1193
H	1.128249	1	109.062371	1	150.927741	1	6	5	4	0.1177
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C6 H8 N10 O16

21-JUN-86

RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,1,1,3,6,8,8,8-octanitro-
3,6-diazaoctane (ONDO)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-24.885196 KCAL
ELECTRONIC ENERGY	=	-58334.699835 EV
CORE-CORE REPULSION	=	50575.680925 EV
DIPOLE	=	0.10187 DEBYE
NO. OF FILLED LEVELS	=	89
IONISATION POTENTIAL	=	11.224387 EV
MOLECULAR WEIGHT	=	476.187
SCF CALCULATIONS	=	17
COMPUTATION TIME	=	********* SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000 RESTART
RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,1,1,3,6,8,8,8-octanitro-
3,6-diazaoctane (ONDO)
C   0.000000 0   0.000000 0   0.000000 0   0 0 0   -0.5394

C	7.906010	1	0.000000	0	0.000000	0	1	0	0	.	-0.5392
C	6.865637	1	9.386801	1	0.000000	0	2	1	0		0.2178
C	6.095307	1	12.369002	1	-2.349168	1	3	2	1		0.2176
C	3.659958	1	7.282490	1	11.755235	1	4	3	2		0.1631
C	1.527651	1	32.460007	1	0.162981	1	5	4	3		0.1620
N	1.511815	1	93.190033	1	115.268594	1	1	2	3		1.1400
N	1.511605	1	88.813106	1	-115.343406	1	2	3	4		1.1398
N	1.538713	1	153.652895	1	-31.504221	1	1	2	3		1.1323
N	1.538932	1	161.668774	1	48.358534	1	2	3	4		1.1323
N	1.525743	1	8\.764813	1	-133.421534	1	1	2	3		1.1264
N	1.525469	1	7\.680229	1	131.711344	1	2	3	4		1.1256
N	1.464049	1	29.605833	1	-91.054464	1	3	2	1		-0.2936
N	1.480219	1	118.454205	1	35.941623	1	6	5	4		-0.2943
N	1.330\.9	1	120.564290	1	-159.015704	1	13	3	2		1.1890
N	1.330348	1	120.125783	1	78.999800	1	14	6	5		1.1892
O	1.220160	1	113.233050	1	19.658232	1	7	1	2		-0.5357
O	1.220159	1	113.267888	1	-10.650833	1	8	2	3		-0.5354
O	1.214396	1	115.083070	1	-158.642153	1	7	1	2		-0.4995
O	1.214470	1	115.049282	1	167.606197	1	8	2	3		-0.4995
O	1.212811	1	114.977429	1	43.171460	1	9	1	2		-0.4866
O	1.212777	1	114.955679	1	-60.723653	1	10	2	3		-0.4865
O	1.216829	1	113.159081	1	-135.677827	1	9	1	2		-0.5076
O	1.216820	1	113.150801	1	118.091134	1	10	2	3		-0.5075
O	1.218163	1	111.942110	1	81.439835	1	11	1	2		-0.5109
O	1.218235	1	111.924058	1	-89.294209	1	12	2	3		-0.5108
O	1.214088	1	116.163867	1	-99.904154	1	11	1	2		-0.4940
O	1.214203	1	116.213013	1	92.052305	1	12	2	3		-0.4945
O	1.226286	1	114.894167	1	-8.135674	1	15	13	3		-0.5702
O	1.226266	1	114.902864	1	169.102995	1	16	14	6		-0.5702
O	1.224911	1	114.248360	1	171.742575	1	15	13	3		-0.5584
O	1.224943	1	114.211746	1	-10.779635	1	16	14	6		-0.5580
H	1.127200	1	79.271475	1	105.121133	1	3	2	1		0.0105
H	1.127079	1	83.313332	1	-107.288230	1	4	3	2		0.0112
H	1.126159	1	122.765583	1	-161.357718	1	3	2	1		0.0274
H	1.126197	1	135.201233	1	156.982712	1	4	3	2		0.0274
H	1.124091	1	108.331718	1	100.163413	1	5	4	3		0.0008
H	1.124161	1	110.878371	1	-88.037439	1	6	5	4		0.0012
H	1.127106	1	79.327560	1	-163.325042	1	5	4	3		-0.0120
H	1.126943	1	110.443357	1	162.764856	1	6	5	4		-0.0097
O	0.000000	0	0.000000	0	0.000000	0	0	0	0		

SUMMARY OF MNDO   CALCULATION

VERSION 3.10

C6 H8 N10 O16

6-JAN-1987 16:53:23

RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,1,1,3,6,8,8,8-octanitro-

3,6-diazaoctane (ONDO)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	225.880243 KCAL
ELECTRONIC ENERGY	=-58245.714854 EV
CORE-CORE REPULSION	= 50172.687999 EV
GRADIENT NORM	=	3.844994
DIPOLE	=	0.34886 DEBYE
NO. OF FILLED LEVELS	=	89
IONISATION POTENTIAL	=	12.748249 EV
MOLECULAR WEIGHT	=	476.187
SCF CALCULATIONS	=	32
COMPUTATION TIME	=	2312.35 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PULAY T=36000
RUN ON POTENTIAL RDX/HMX REPLACEMENT 1,1,1,3,6,8,8,8-octanitro-
3,6-diazaoctane (ONDO)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0498
C	8.150737	1	0.000000	0	0.000000	0	1	0	0	0.0507
C	7.012891	1	8.341337	1	0.000000	0	2	1	0	0.1495
C	6.145116	1	11.557040	1	5.096087	1	3	2	1	0.1463
C	3.691454	1	7.533681	1	13.173049	1	4	3	2	0.1225
C	1.559020	1	33.025862	1	13.394930	1	5	4	3	0.1316
N	1.574907	1	123.416839	1	90.337310	1	1	2	3	0.4412
N	1.571390	1	116.809027	1	-97.937347	1	2	3	4	0.4395
N	1.579902	1	130.913364	1	-71.304352	1	1	2	3	0.4339
N	1.583289	1	137.359222	1	80.142150	1	2	3	4	0.4400
N	1.567057	1	72.399184	1	-170.132505	1	1	2	3	0.4535
N	1.568943	1	63.736972	1	162.651941	1	2	3	4	0.4457
N	1.480813	1	30.383063	1	-56.832121	1	3	2	1	-0.3776
N	1.505473	1	110.684147	1	31.284983	1	6	5	4	-0.3752
N	1.444633	1	115.671958	1	-132.248269	1	13	3	2	0.5511
N	1.435258	1	113.494018	1	92.268613	1	14	6	5	0.5625
O	1.202821	1	118.564326	1	-25.827306	1	7	1	2	-0.2661
O	1.202712	1	118.541403	1	-16.150636	1	8	2	3	-0.2509
O	1.203107	1	118.024039	1	154.576854	1	7	1	2	-0.2472
O	1.204028	1	118.104138	1	161.932881	1	8	2	3	-0.2601
O	1.205929	1	116.975757	1	88.377567	1	9	1	2	-0.2795
O	1.203000	1	118.639502	1	-77.541630	1	10	2	3	-0.2623
O	1.200675	1	119.536843	1	-92.983419	1	9	1	2	-0.2328
O	1.202715	1	117.839050	1	102.973644	1	10	2	3	-0.2492
O	1.205405	1	117.401292	1	67.089696	1	11	1	2	-0.2807
O	1.207604	1	116.547246	1	-63.741800	1	12	2	3	-0.2984
O	1.201798	1	119.156765	1	-111.321241	1	11	1	2	-0.2471
O	1.200212	1	120.231781	1	117.953226	1	12	2	3	-0.2289
O	1.204361	1	119.642210	1	58.129604	1	15	13	3	-0.2887
O	1.206248	1	119.510721	1	114.527087	1	16	14	6	-0.3102
O	1.200354	1	115.002493	1	-122.605057	1	15	13	3	-0.2484

O	1.201367	1	116.130504	1	-67.512559	1	16	14	6	-0.2575
H	1.119360	1	80.242918	1	104.594392	1	3	2	1	0.0746
H	1.119097	1	78.547022	1	-104.293172	1	4	3	2	0.0805
H	1.118619	1	114.290008	1	-152.838569	1	3	2	1	0.0877
H	1.119070	1	130.198205	1	155.543338	1	4	3	2	0.0916
H	1.114938	1	109.694740	1	110.462368	1	5	4	3	0.0554
H	1.115112	1	110.316759	1	-88.989516	1	6	5	4	0.0492
H	1.115485	1	80.171522	1	-146.357664	1	5	4	3	0.0525
H	1.116408	1	110.725726	1	154.353753	1	6	5	4	0.0515
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

RDX.ARC
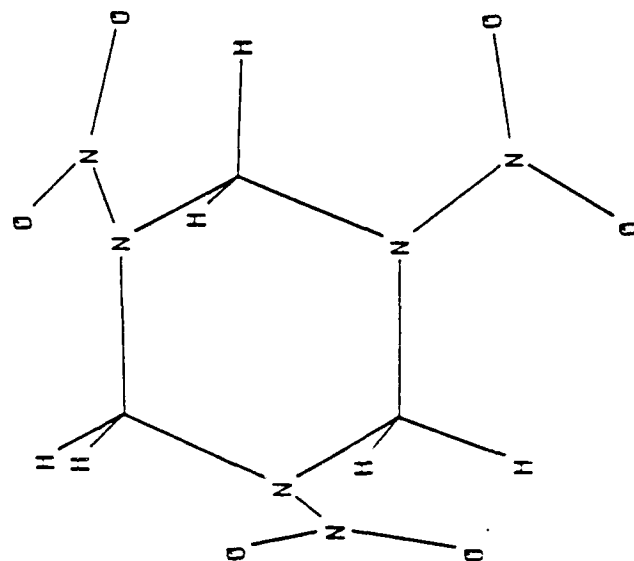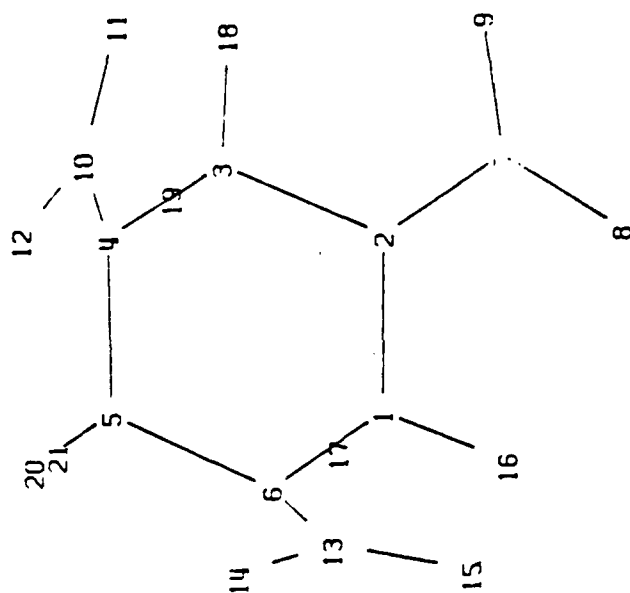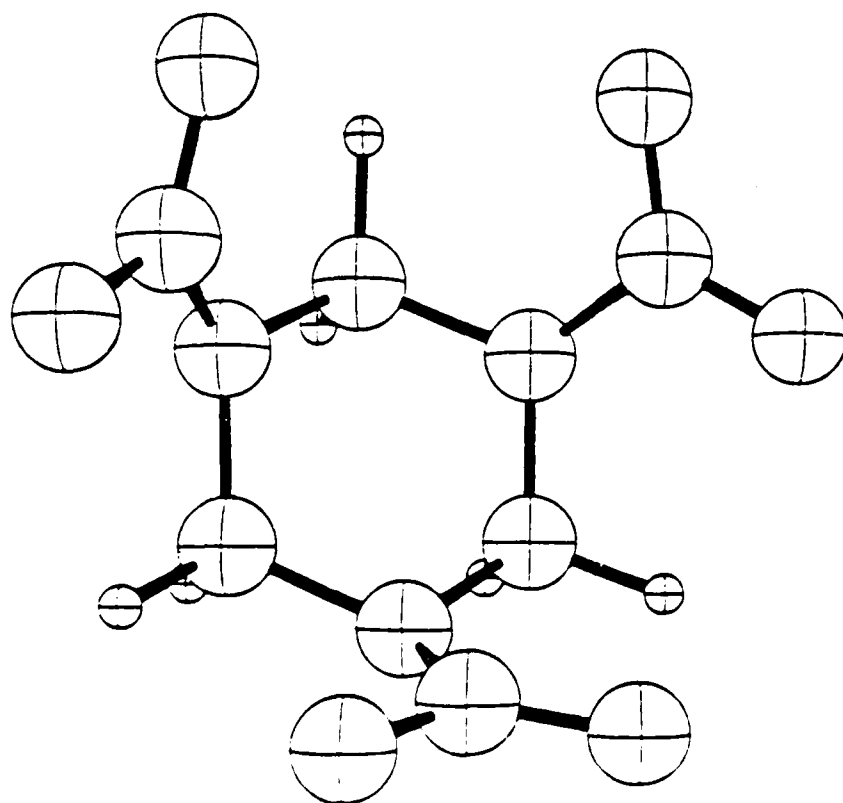
Figure A-12. 1,3,5-Trinitro-1,3,5-triazacyclohexane
[Ref. A-11].

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VERSION 3.00

C3   H6   N6   O6

25-FEB-86

AM1
RUN ON 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	105.124442 KCAL
ELECTRONIC ENERGY	=	-19056.557001 EV
CORE-CORE REPULSION	=	15438.562786 EV
DIPOLE	=	6.98385 DEBYE
NO. OF FILLED LEVELS	=	42
IONISATION POTENTIAL	=	12.104123 EV
MOLECULAR WEIGHT	=	222.117
SCF CALCULATIONS	=	71
COMPUTATION TIME	=	40015.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 AM1 RESTART
AM1
RUN ON 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX)

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0155
N	1.473805	1	0.000000	0	0.000000	0	1	0	0	-0.3336
C	1.474329	1	112.795893	1	0.000000	0	2	1	0	0.0159
N	1.474707	1	115.781397	1	45.813823	1	3	2	1	-0.3332
C	1.474135	1	112.613350	1	-46.012353	1	4	3	2	0.0154
N	1.473855	1	115.897913	1	45.883071	1	5	4	3	-0.3331
N	1.417118	1	118.254100	1	98.471918	1	2	1	6	0.6093
O	1.198718	1	117.716192	1	21.191208	1	7	2	1	-0.3216
O	1.198663	1	117.677651	1	-21.753235	1	7	2	3	-0.3211
N	1.416859	1	118.260806	1	97.733149	1	4	3	2	0.6092
O	1.198706	1	117.700487	1	21.469669	1	10	4	3	-0.3213
O	1.198762	1	117.693385	1	-21.595847	1	10	4	5	-0.3214
N	1.417688	1	118.183605	1	98.318693	1	6	5	4	0.6089
O	1.198722	1	117.690507	1	21.769291	1	13	6	5	-0.3211
O	1.198759	1	117.713295	1	-21.169067	1	13	6	1	-0.3215
H	1.136643	1	110.562069	1	171.939606	1	1	6	5	0.1964
H	1.133370	1	105.126573	1	-70.421163	1	1	6	5	0.1550
H	1.136233	1	110.526045	1	172.538350	1	3	2	1	0.1963
H	1.133374	1	105.164985	1	-69.751417	1	3	2	1	0.1549
H	1.136389	1	110.521897	1	172.714783	1	5	4	3	0.1963
H	1.133514	1	105.118128	1	-69.659737	1	5	4	3	0.1549
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

VERSION 3.00

C3 H6 N6 O6

20-FEB-86

MINDO/3
RUN ON 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-34.517795 KCAL
ELECTRONIC ENERGY	=	-18468.821823 EV
CORE-CORE REPULSION	=	14985.721788 EV
DIPOLE	=	6.48204 DEBYE
NO. OF FILLED LEVELS	=	42
IONISATION POTENTIAL	=	10.719884 EV
MOLECULAR WEIGHT	=	222.117
SCF CALCULATIONS	=	51
COMPUTATION TIME	=	3017.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 MINDO3
MINDO/3
RUN ON 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3077
N	1.457599	1	0.000000	0	0.000000	0	1	0	0	-0.3483
C	1.455492	1	112.030285	1	0.000000	0	2	1	0	0.3079
N	1.457233	1	106.184431	1	60.969738	1	3	2	1	-0.3487
C	1.455731	1	112.089913	1	-60.887985	1	4	3	2	0.3080
N	1.457319	1	106.143496	1	60.803272	1	5	4	3	-0.3488
N	1.325554	1	123.885162	1	117.895340	1	2	1	6	1.1934
O	1.226069	1	114.337323	1	-19.059322	1	7	2	1	-0.5711
O	1.225069	1	114.712106	1	-20.612638	1	7	2	3	-0.5638
N	1.325754	1	123.888170	1	118.300086	1	4	3	2	1.1936
O	1.225962	1	114.335246	1	-19.787316	1	10	4	3	-0.5706
O	1.225078	1	114.688230	1	-21.028920	1	10	4	5	-0.5639
N	1.325793	1	123.867204	1	118.149983	1	6	5	4	1.1936
O	1.225999	1	114.319824	1	-20.104085	1	13	6	5	-0.5707
O	1.225044	1	114.691255	1	-21.436971	1	13	6	1	-0.5637
H	1.125688	1	116.000599	1	-170.011521	1	1	6	5	0.0256
H	1.138512	1	110.614505	1	-57.788882	1	1	6	5	-0.0436
H	1.125726	1	115.984566	1	-170.062429	1	3	2	1	0.0255
H	1.138570	1	110.552551	1	-57.910323	1	3	2	1	-0.0438
H	1.125743	1	115.990748	1	-170.299099	1	5	4	3	0.0253

| H | 1.138536 | 1 | 110.597062 | 1 | -58.068916 | 1 | 5 | 4 | 3 | -0.0437 |
| O | 0.000000 | 0 | 0.000000 | 0 | 0.000000 | 0 | 0 | 0 | 0 | |

SUMMARY OF   MNDO   CALCULATION

VERSION   3.00

C3   H6   N6   O6

20-FEB-86

MNDO
RUN ON 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	102.772209 KCAL
ELECTRONIC ENERGY	=-19030.800113 EV
CORE-CORE REPULSION	= 15398.935703 EV
DIPOLE	=	6.83599 DEBYE
NO. OF FILLED LEVELS	=	42
IONISATION POTENTIAL	=	12.287845 EV
MOLECULAR WEIGHT	=	222.117
SCF CALCULATIONS	=	424
COMPUTATION TIME	= 32936.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000
MNDO
RUN ON 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3089
N	1.485785	1	0.000000	0	0.000000	0	1	0	0	-0.4488
C	1.484341	1	115.571571	1	0.000000	0	2	1	0	0.3100
N	1.485665	1	109.959412	1	50.910323	1	3	2	1	-0.4492
C	1.484179	1	115.599155	1	-50.963036	1	4	3	2	0.3092
N	1.485703	1	110.031481	1	50.778360	1	5	4	3	-0.4471
N	1.411950	1	119.757504	1	101.414720	1	2	1	6	0.5916
O	1.206966	1	118.692501	1	-22.593670	1	7	2	1	-0.3188
O	1.203835	1	116.727130	1	-54.700078	1	7	2	3	-0.2818
N	1.411963	1	119.769171	1	101.375371	1	4	3	2	0.5921
O	1.206895	1	118.698830	1	-22.375567	1	10	4	3	-0.3181
O	1.203941	1	116.710053	1	-54.364043	1	10	4	5	-0.2826
N	1.413591	1	119.578486	1	100.914944	1	6	5	4	0.5897
O	1.206899	1	118.737518	1	-24.410578	1	13	6	5	-0.3179
O	1.203695	1	116.637866	1	-57.038440	1	13	6	1	-0.2801
H	1.116587	1	113.127661	1	177.460570	1	1	6	5	0.0896

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H     1.124443  1  107.462718  1   -65.579637  1  1  6  5       0.0581
H     1.116491  1  113.172425  1   177.772639  1  3  2  1       0.0902
H     1.124467  1  107.489596  1   -65.231913  1  3  2  1       0.0577
H     1.116581  1  113.240346  1   177.588054  1  5  4  3       0.0896
H     1.124464  1  107.499087  1   -65.356867  1  5  4  3       0.0580
0     0.000000  0    0.000000  0     0.000000  0  0  0  0
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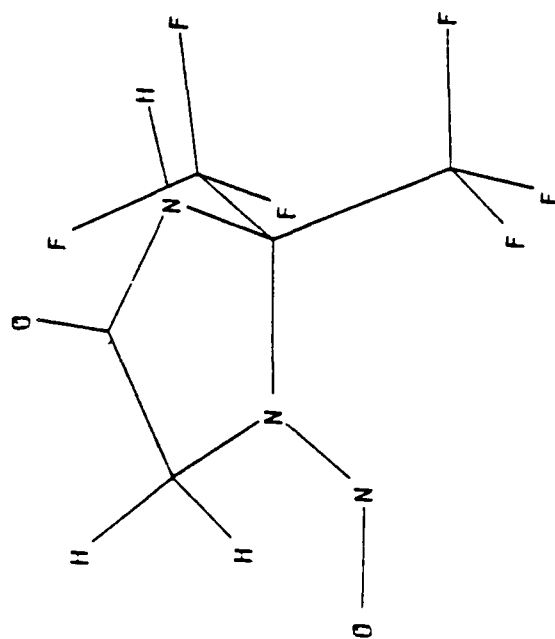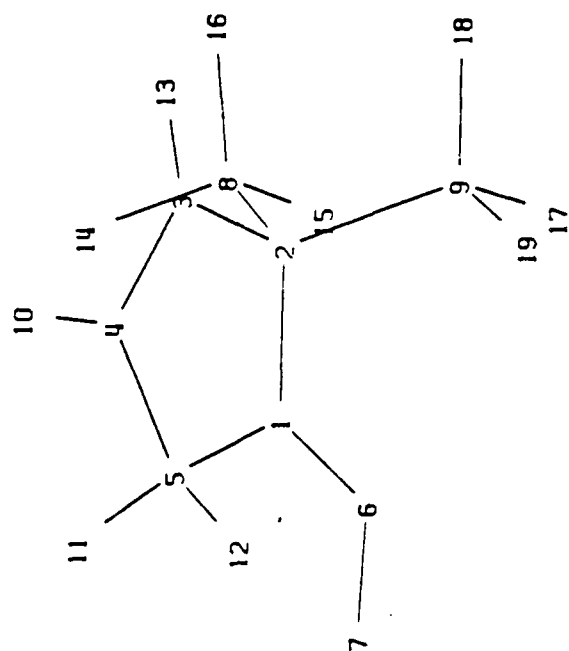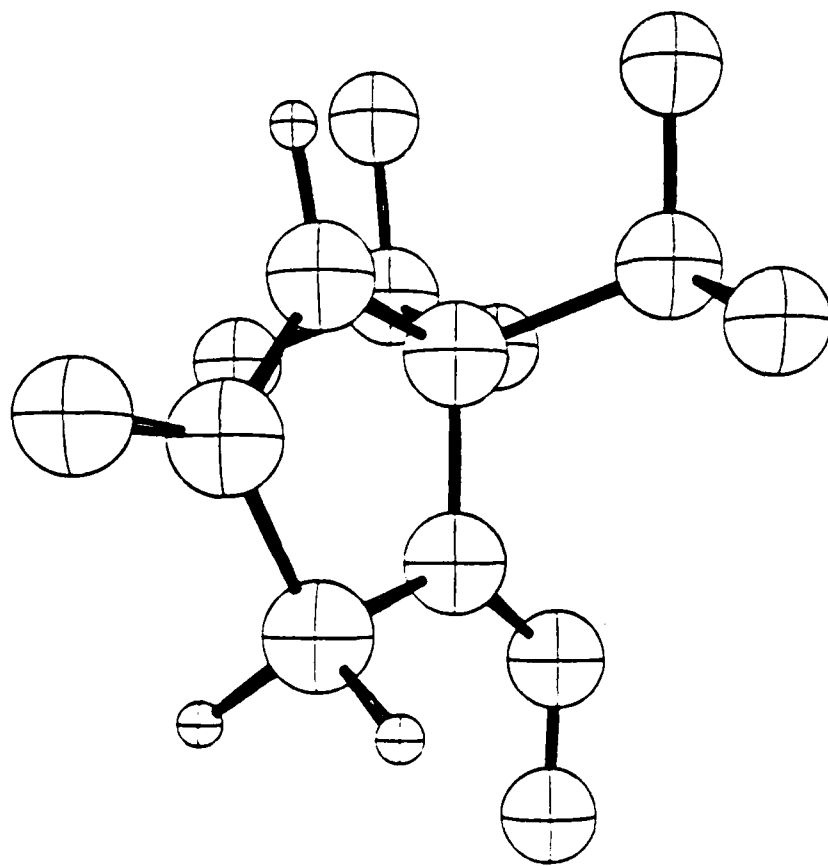
Figure A-13. 1-Nitroso-2,2-di(trifluoromethyl)-1,3-diazacyclopentan-4-one [Ref. A-12].

SCEC2A.ARC

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SUMMARY OF   AM1   CALCULATION

C5   H3   N3   O2   F6

29-JUL-86

AM1
1-Nitroso-2,2-di(trifluoromethyl)-1,3-diazacyclopentan-4-one

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-308.264595 KCAL
ELECTRONIC ENERGY	=	-23015.151924 EV
CORE-CORE REPULSION	=	18161.740602 EV
DIPOLE	=	0.85386 DEBYE
NO. OF FILLED LEVELS	=	46
IONISATION POTENTIAL	=	11.257546 EV
MOLECULAR WEIGHT	=	251.088
SCF CALCULATIONS	=	133
COMPUTATION TIME	=	14781.86 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 AM1
AM1
1-Nitroso-2,2-di(trifluoromethyl)-1,3-diazacyclopentan-4-one

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.3645
C	1.476787	1	0.000000	0	0.000000	0	1	0	0	0.1619
N	1.446706	1	106.523452	1	0.000000	0	2	1	0	-0.4051
C	1.402121	1	111.716841	1	-0.371656	1	3	2	1	0.3207
C	1.535622	1	107.541248	1	0.231165	1	4	3	2	-0.0794
N	1.339540	1	122.204469	1	-177.919821	1	1	2	3	0.3403
O	1.159094	1	90.384290	1	178.346097	1	6	5	4	-0.2266
C	1.617636	1	110.995896	1	61.553108	1	2	1	6	0.3995
C	1.617433	1	111.263953	1	-57.315458	1	2	1	6	0.3998
O	1.229670	1	124.850273	1	-179.773450	1	4	3	2	-0.2798
H	1.123548	1	110.299003	1	60.738031	1	5	4	10	0.1480
H	1.123559	1	110.327467	1	-60.546667	1	5	4	10	0.1477
H	0.989234	1	121.405311	1	-179.721583	1	3	2	1	0.2841
F	1.366114	1	112.845259	1	176.637233	1	8	2	9	-0.1431
F	1.363681	1	113.575839	1	56.151687	1	8	2	9	-0.1327
F	1.367786	1	112.160018	1	-64.177542	1	8	2	9	-0.1476
F	1.363738	1	113.555627	1	-54.064393	1	9	2	8	-0.1329
F	1.367778	1	112.265953	1	66.209134	1	9	2	8	-0.1471
F	1.366166	1	112.822988	1	-174.536503	1	9	2	8	-0.1431
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

VERSION 3.10

C5   H3   N3   O2   F6

7-AUG-1986 23:19:38

MINDO/3
1-Nitroso-2,2-di(trifluoromethyl)-1,3-diazacyclopentan-4-one

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-432.374941 KCAL
ELECTRONIC ENERGY	=	-23997.437387 EV
CORE-CORE REPULSION	=	19248.551060 EV
DIPOLE	=	0.74139 DEBYE
NO. OF FILLED LEVELS	=	46
IONISATION POTENTIAL	=	9.355227 EV
MOLECULAR WEIGHT	=	251.088
SCF CALCULATIONS	=	694
COMPUTATION TIME	=	8007.32 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 MINDO
MINDO/3
1-Nitroso-2,2-di(trifluoromethyl)-1,3-diazacyclopentan-4-one

Atom											CHARGE
N	0.000000	0	0.000000	0	0.000000	0	0	0	0		-0.1725
C	1.477815	1	0.000000	0	0.000000	0	1	0	0		0.0233
N	1.426954	1	101.211915	1	0.000000	0	2	1	0		-0.2447
C	1.384500	1	117.052671	1	12.131195	1	3	2	1		0.6291
C	1.510288	1	104.044819	1	-2.651157	1	4	3	2		-0.0036
N	1.280897	1	115.012267	1	156.282918	1	1	2	3		0.6550
O	1.205093	1	99.309420	1	-158.653618	1	6	5	4		-0.4457
C	1.523649	1	109.828446	1	26.764049	1	2	1	6		1.1411
C	1.540772	1	114.068279	1	-78.958310	1	2	1	6		1.2467
O	1.203445	1	123.237372	1	178.371793	1	4	3	2		-0.4933
H	1.121422	1	111.619064	1	47.797989	1	5	4	10		0.0354
H	1.123468	1	111.323610	1	-66.740983	1	5	4	10		0.0280
H	1.023709	1	116.870721	1	-170.237198	1	3	2	1		0.1224
F	1.329817	1	125.696462	1	-145.145992	1	8	2	9		-0.4230
F	1.349149	1	89.576898	1	96.542042	1	8	2	9		-0.4002
F	1.357457	1	80.273699	1	-29.241058	1	8	2	9		-0.4038
F	1.361563	1	75.200484	1	-42.651040	1	9	2	8		-0.4597
F	1.322440	1	118.459379	1	74.282259	1	9	2	8		-0.3658
F	1.327937	1	114.545781	1	-158.037833	1	9	2	8		-0.4686
O	0.000000	0	0.000000	0	0.000000	0	0	0	0		

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C5 H3 N3 O2 F6

MNDO
1-Nitroso-2,2-di(trifluoromethyl)-1,3-diazacyclopentan-4-one

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   -314.736516 KCAL
ELECTRONIC ENERGY   =-22932.408406 EV
CORE-CORE REPULSION   = 18108.345300 EV
DIPOLE   =   1.71901 DEBYE
NO. OF FILLED LEVELS   =   46
IONISATION POTENTIAL   =   11.839674 EV
MOLECULAR WEIGHT   =   251.088
SCF CALCULATIONS   =   222
COMPUTATION TIME   =   1668.20 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000
MNDO
1-Nitroso-2,2-di(trifluoromethyl)-1,3-diazacyclopentan-4-one

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.4490
C	1.469037	1	0.000000	0	0.000000	0	1	0	0	0.2777
N	1.442923	1	102.914295	1	0.000000	0	2	1	0	-0.4548
C	1.419054	1	114.399571	1	-0.873267	1	3	2	1	0.3529
C	1.528954	1	106.833200	1	0.985117	1	4	3	2	0.1507
N	1.362248	1	118.905105	1	-177.866765	1	1	2	3	0.3064
O	1.159393	1	90.062486	1	178.870703	1	6	5	4	-0.1779
C	1.649949	1	110.651610	1	64.798507	1	2	1	6	0.5803
C	1.649607	1	111.137314	1	-60.823808	1	2	1	6	0.5827
O	1.216255	1	122.029137	1	-179.334481	1	4	3	2	-0.2729
H	1.115336	1	111.384400	1	60.464072	1	5	4	10	0.0641
H	1.115124	1	111.335979	1	-60.763813	1	5	4	10	0.0641
H	1.001841	1	122.161706	1	-177.548720	1	3	2	1	0.2413
F	1.352812	1	111.208383	1	178.087209	1	8	2	9	-0.2135
F	1.349751	1	113.284890	1	57.822349	1	8	2	9	-0.2043
F	1.352823	1	111.632345	1	-62.819049	1	8	2	9	-0.2152
F	1.350104	1	113.250336	1	-53.909237	1	9	2	8	-0.2053
F	1.352915	1	111.635452	1	66.667935	1	9	2	8	-0.2144
F	1.352659	1	111.241000	1	-174.176680	1	9	2	8	-0.2129
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SLECiC.ARC
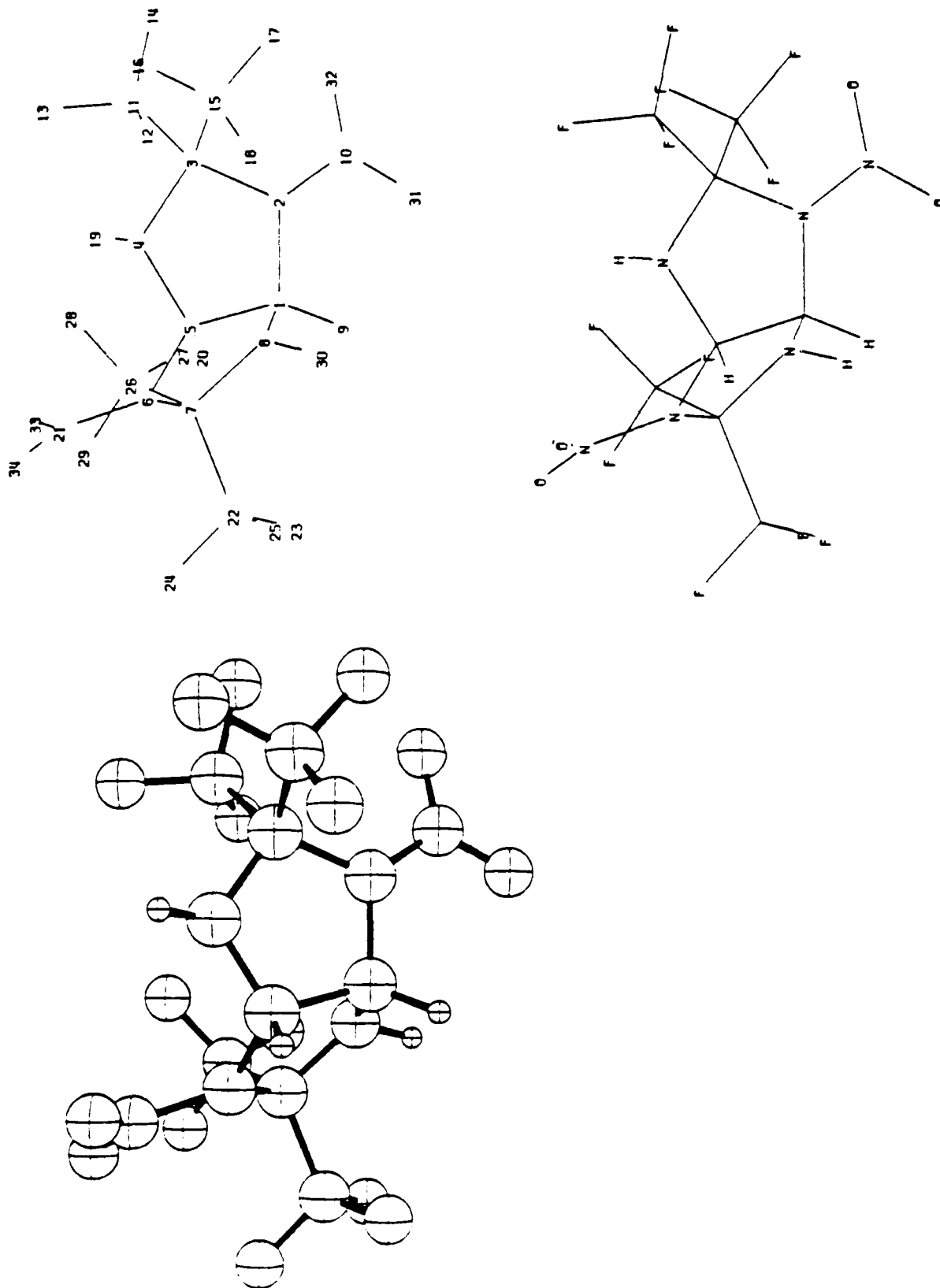
Figure A-14. 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-
2,4,6,8-tetraazabicyclo[3.3.0]octane [Refs. A-12 and A-13].

C8   H4   N6   O4   F12

AM1 // 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-2,4,6,8-tetraazabicyclo[3.3.0]octane

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-697.632390 KCAL
ELECTRONIC ENERGY	=-63524.904610 EV
CORE-CORE REPULSION	= 54165.610535 EV
GRADIENT NORM	=	36.626840
DIPOLE	=	3.28787 DEBYE
NO. OF FILLED LEVELS	=	87
IONISATION POTENTIAL	=	11.893958 EV
MOLECULAR WEIGHT	=	476.138
SCF CALCULATIONS	=	175
COMPUTATION TIME	= 77417.39 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 SHIFT=30 RESTART
AM1 // 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-2,4,6,8-tetraazabicyclo[3.3.0]octane

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0965
N	1.490835	1	0.000000	0	0.000000	0	1	0	0	-0.3346
C	1.475453	1	109.372338	1	0.000000	0	2	1	0	0.0821
N	1.448328	1	108.247055	1	8.498409	1	3	2	1	-0.3559
C	1.448366	1	111.592537	1	-3.217792	1	4	3	2	0.1313
N	1.495486	1	103.463829	1	135.545011	1	5	1	2	-0.3757
C	1.470960	1	110.251624	1	23.333534	1	6	5	2	0.0918
N	1.446192	1	108.006903	1	-0.757296	1	7	6	5	-0.3575
H	1.130188	1	106.227722	1	-128.725768	1	1	2	3	0.1779
N	1.409746	1	118.907689	1	-160.742647	1	2	1	5	0.6571
C	1.693907	1	114.833998	1	-116.768736	1	3	2	1	0.5582
F	1.321562	1	109.538882	1	36.676586	1	11	3	2	-0.2001
F	1.323703	1	110.153548	1	155.086839	1	11	3	2	-0.2009
F	1.315866	1	112.029864	1	-84.462045	1	11	3	2	-0.1757
C	1.706416	1	106.817209	1	123.001551	1	3	2	1	0.5949
F	1.319018	1	109.422452	1	177.638265	1	15	3	2	-0.1941
F	1.317709	1	111.129021	1	56.897538	1	15	3	2	-0.1865
F	1.320457	1	110.128516	1	-62.858520	1	15	3	2	-0.1938
H	0.998690	1	117.804084	1	-148.354705	1	4	3	2	0.2741
H	1.131998	1	108.176957	1	118.020797	1	5	4	3	0.1921
N	1.402907	1	120.285134	1	-163.319185	1	6	5	1	0.6544
C	1.701726	1	107.631878	1	117.850577	1	7	6	5	0.5551
F	1.324317	1	109.036313	1	-64.991899	1	22	7	6	-0.2087

F	1.315173	1	112.283926	1	55.102546	1	22	7	6	-0.1769
F	1.320642	1	109.524710	1	176.936525	1	22	7	6	-0.1985
C	1.695338	1	114.591256	1	-121.463629	1	7	6	5	0.5888
F	1.319384	1	110.933649	1	158.497494	1	26	7	6	-0.1843
F	1.321104	1	109.022807	1	38.892315	1	26	7	6	-0.2010
F	1.317342	1	111.153806	1	-81.076963	1	26	7	6	-0.1814
H	0.999636	1	116.315831	1	147.103390	1	8	7	6	0.2667
O	1.198219	1	115.585122	1	-23.547824	1	10	2	1	-0.3167
O	1.192565	1	118.829282	1	160.806756	1	10	2	1	-0.2834
O	1.199295	1	115.899370	1	-10.278847	1	21	6	5	-0.3202
O	1.192397	1	118.679898	1	172.877129	1	21	6	5	-0.2750
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.10

C8 H4 N6 O4 F12

31--DEC-86

MINDO/3 // 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-2,4,6,8-tetraazabicyclo[3.3.0]octane

PETERS TEST WAS SATISFIED IN FLETCHER-POWELL OPTIMISATION
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-928.156265 KCAL
ELECTRONIC ENERGY	=	-67910.4G7017 EV
CORE-CORE REPULSION	=	58693.173937 EV
GRADIENT NORM	=	2.647270
DIPOLE	=	1.06556 DEBYE
NO. OF FILLED LEVELS	=	87
IONISATION POTENTIAL	=	9.002895 EV
MOLECULAR WEIGHT	=	476.138
SCF CALCULATIONS	=	14
COMPUTATION TIME	=	2887.25 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PULAY MINDO T=36000 SCFCRT=0.01 GNORM=7.5
MINDO/3 // 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-2,4,6,8-tetraazabicyclo[3.3.0]octane

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.2457
N	1.504831	1	0.000000	0	0.000000	0	1	0	0	-0.4332
C	1.395697	1	108.011611	1	0.000000	0	2	1	0	0.7553
N	1.351171	1	110.402809	1	10.158743	1	3	2	1	-0.3601
C	1.440306	1	112.955264	1	-4.824509	1	4	3	2	0.2355
N	1.470863	1	105.151581	1	124.153122	1	5	1	2	-0.3578

C	1.486069	1	109.144543	1	19.108581	1	6	5	2	0.1635
N	1.446366	1	103.165471	1	19.225847	1	7	6	5	-0.2909
H	1.132293	1	109.997297	1	-132.863700	1	1	2	3	0.0019
N	1.323928	1	126.656531	1	171.318932	1	2	1	5	1.2135
C	2.797124	1	117.056493	1	-82.686637	1	3	2	1	1.1350
F	1.326607	1	105.855585	1	-28.690038	1	11	3	2	-0.3909
F	1.575251	1	55.211425	1	157.187297	1	11	3	2	-0.5384
F	1.497385	1	18.992085	1	-94.792421	1	11	3	2	-0.4478
C	2.367560	1	152.776079	1	-136.202612	1	3	2	1	1.0743
F	1.287050	1	99.640788	1	-106.878561	1	15	3	2	-0.4659
F	1.395499	1	111.482854	1	57.730605	1	15	3	2	-0.5043
F	1.493817	1	32.223446	1	-93.379999	1	15	3	2	-0.1971
H	1.111277	1	107.475028	1	-151.534309	1	4	3	2	0.2669
H	1.132389	1	111.869411	1	118.092322	1	5	4	3	0.0117
N	1.315476	1	125.099172	1	162.511272	1	6	5	1	1.2139
C	1.580495	1	114.723498	1	131.699593	1	7	6	5	1.2700
F	1.333185	1	94.291202	1	-17.843615	1	22	7	6	-0.5333
F	1.301298	1	124.202110	1	118.103169	1	22	7	6	-0.3293
F	1.368048	1	85.893031	1	-126.124207	1	22	7	6	-0.5394
C	1.504487	1	111.683058	1	-103.147905	1	7	6	5	0.7630
F	1.395543	1	68.764773	1	-116.361196	1	26	7	6	-0.3605
F	1.320812	1	138.343465	1	117.559442	1	26	7	6	-0.1705
F	1.387527	1	116.826662	1	21.724145	1	26	7	6	-0.3886
H	1.075796	1	108.043853	1	129.937712	1	8	7	6	0.2568
O	1.223278	1	114.764015	1	3.422071	1	10	2	1	-0.5664
O	1.224310	1	113.265553	1	-175.761933	1	10	2	1	-0.5686
O	1.226432	1	114.525284	1	-12.224506	1	21	6	5	-0.5787
O	1.227292	1	114.038562	1	164.352255	1	21	6	5	-0.5854
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF   MNDO   CALCULATION

VERSION 3.00

C8   H4   N6   O4   F12

MNDO // 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-2,4,6,8-tetraazabicyclo[3.3.0]octane

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   = -474.021947 KCAL
ELECTRONIC ENERGY   =-63230.059464 EV
CORE-CORE REPULSION   = 53872.827650 EV

GRADIENT NORM   =   7.743327
DIPOLE   =   4.23941 DEBYE
NO. OF FILLED LEVELS   =   87
IONISATION POTENTIAL   =   12.534832 EV
MOLECULAR WEIGHT   =   476.138
SCF CALCULATIONS   =   86
COMPUTATION TIME   = 78127.74 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 SHIFT=75 RESTART
MNDO // 2,6-Dinitro-3,3,7,7-tetra(trifluoromethyl)-2,4,6,8-
tetraazabicyclo[3.3.0]octane

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.2622
N	1.492949	1	0.000000	0	0.000000	0	1	0	0	-0.4235
C	1.482025	1	112.382887	1	0.000000	0	2	1	0	0.2225
N	1.462408	1	103.136029	1	1.283121	1	3	2	1	-0.3922
C	1.461617	1	113.643529	1	10.088429	1	4	3	2	0.2623
N	1.495499	1	103.603087	1	133.860950	1	5	1	2	-0.4165
C	1.480029	1	112.486028	1	21.953497	1	6	5	2	0.2204
N	1.462676	1	103.096348	1	0.916013	1	7	6	5	-0.3917
H	1.122049	1	108.915586	1	-132.771895	1	1	2	3	0.0962
N	1.410650	1	119.540994	1	-172.780831	1	2	1	5	0.6219
C	1.654135	1	116.706723	1	-114.723342	1	3	2	1	0.6146
F	1.347994	1	111.608670	1	29.430016	1	11	3	2	-0.2010
F	1.350963	1	111.325008	1	149.348523	1	11	3	2	-0.2015
F	1.350197	1	112.585892	1	-91.431420	1	11	3	2	-0.2010
C	1.659217	1	107.255107	1	118.818820	1	3	2	1	0.5780
F	1.351833	1	111.386144	1	-179.348005	1	15	3	2	-0.2092
F	1.346816	1	113.475464	1	59.317286	1	15	3	2	-0.1928
F	1.354692	1	110.883398	1	-60.754169	1	15	3	2	-0.2198
H	1.008515	1	115.605526	1	146.337634	1	4	3	2	0.2106
H	1.120831	1	112.417770	1	107.333465	1	5	4	3	0.0963
N	1.412125	1	119.103481	1	-171.053313	1	6	5	1	0.6192
C	1.660478	1	107.025491	1	118.398993	1	7	6	5	0.5768
F	1.354644	1	110.981844	1	-61.540416	1	22	7	6	-0.2198
F	1.346661	1	113.352498	1	58.544218	1	22	7	6	-0.1934
F	1.351945	1	111.433547	1	179.819592	1	22	7	6	-0.2093
C	1.651680	1	117.702604	1	-115.075950	1	7	6	5	0.6152
F	1.351133	1	111.512295	1	151.921822	1	26	7	6	-0.2016
F	1.348994	1	111.206088	1	32.448021	1	26	7	6	-0.2022
F	1.350264	1	112.895976	1	-88.470908	1	26	7	6	-0.1997
H	1.008421	1	115.780059	1	146.861172	1	8	7	6	0.2103
O	1.205343	1	116.251487	1	-24.984709	1	10	2	1	-0.2956
O	1.201012	1	118.807405	1	158.441037	1	10	2	1	-0.2703
O	1.205418	1	116.165253	1	-26.303746	1	21	6	5	-0.2950
O	1.200940	1	118.890697	1	157.528197	1	21	6	5	-0.2702
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

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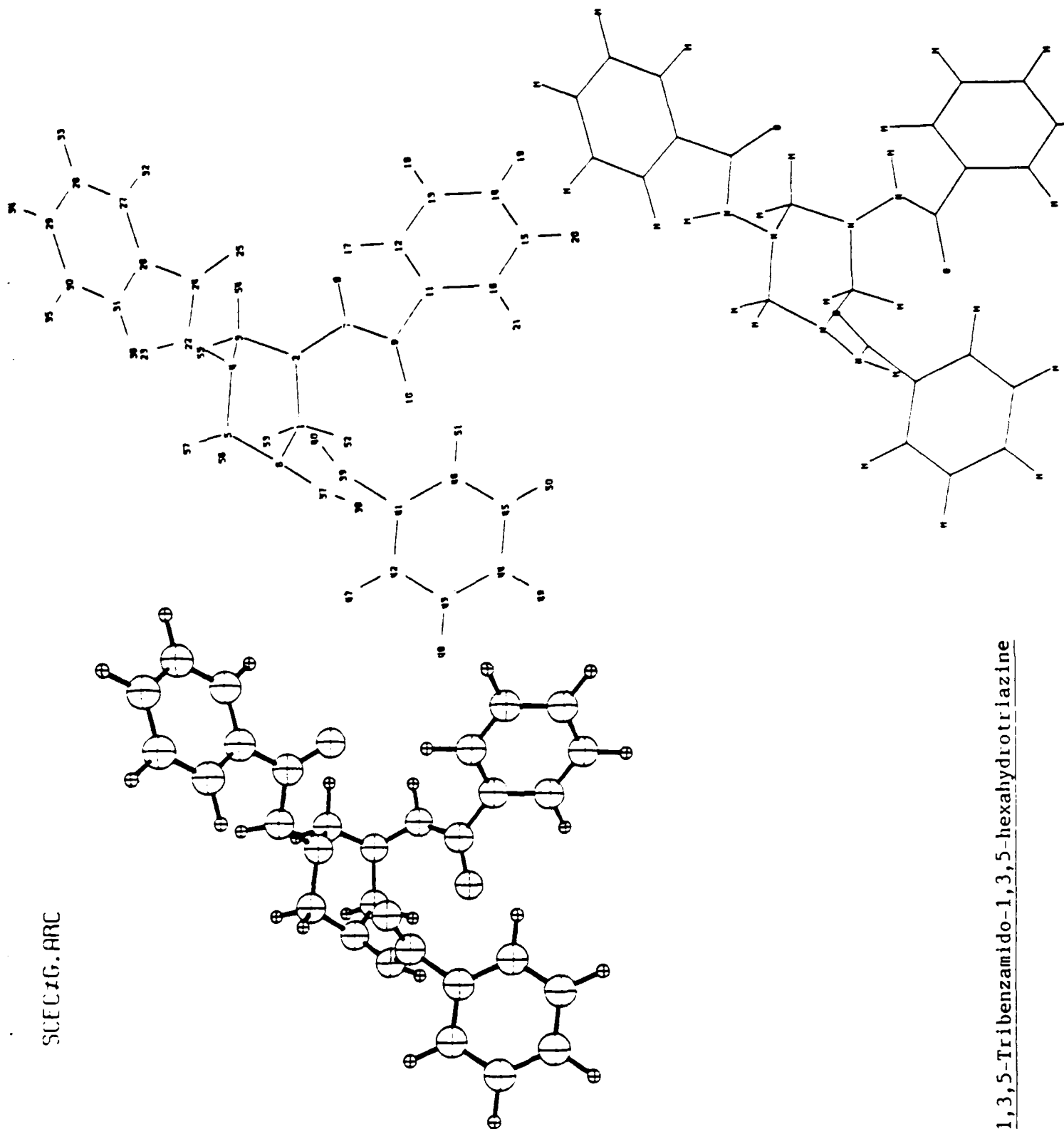
Figure A-15. 1,3,5-Tribenzamido-1,3,5-hexahydrotriazine [Ref. A-12].

C24 H24 N6   O3

AM1
1,3,5-Tribenazmido-1,3,5-hexahydrotriazine monohydrate

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	110.936232 KCAL
ELECTRONIC ENERGY	=-48971.410985 EV
CORE-CORE REPULSION	= 43371.163107 EV
GRADIENT NORM	=	6.920331
DIPOLE	=	3.50857 DEBYE
NO. OF FILLED LEVELS	=	84
IONISATION POTENTIAL	=	8.711320 EV
MOLECULAR WEIGHT	=	444.492
SCF CALCULATIONS	=	29
COMPUTATION TIME	=106029.08 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 AM1 RESTART
AM1
1,3,5-Tribenazmido-1,3,5-hexahydrotriazine monohydrate

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0412
N	1.482950	1	0.000000	0	0.000000	0	1	0	0	-0.1205
C	1.489980	1	109.715352	1	0.000000	0	2	1	0	-0.0918
N	1.488662	1	112.623639	1	51.476299	1	3	2	1	-0.1728
C	1.493571	1	108.603624	1	-62.636281	1	4	3	2	0.0022
N	1.477876	1	114.681837	1	57.116668	1	5	4	3	-0.1505
N	1.371223	1	117.981667	1	97.035894	1	2	1	6	-0.2649
H	1.008947	1	110.094127	1	-176.521939	1	7	2	1	0.2248
C	1.410134	1	127.664291	1	-32.150671	1	7	2	1	0.3345
O	1.245483	1	122.002134	1	31.384785	1	9	7	2	-0.3769
C	1.489595	1	115.530361	1	-155.270923	1	9	7	2	-0.1361
C	1.399211	1	119.903855	1	-127.430229	1	11	9	10	-0.0973
C	1.395148	1	119.507771	1	178.522434	1	12	11	9	-0.1345
C	1.395615	1	120.170338	1	0.172639	1	13	12	11	-0.1090
C	1.395231	1	-120.084440	1	-0.265215	1	14	13	12	-0.1428
C	1.393805	1	120.174550	1	-0.100803	1	15	14	13	-0.0831
H	1.105104	1	119.879116	1	178.603578	1	12	13	14	0.1706
H	1.100090	1	120.181683	1	179.397286	1	13	14	15	0.1409
H	1.100112	1	119.950526	1	179.722021	1	14	15	16	0.1335
H	1.099898	1	119.790995	1	-179.762676	1	15	16	11	0.1352
H	1.100664	1	119.757716	1	179.017762	1	16	11	12	0.1454
N	1.367409	1	115.964920	1	168.230533	1	4	3	2	-0.2688
H	1.006886	1	116.505542	1	74.146308	1	22	4	3	0.1909

C	1.416872	1	120.296496	1	-71.385366	1	22	4	3	0.3569
O	1.242790	1	123.575832	1	0.964746	1	24	22	4	-0.3387
C	1.490665	1	114.478613	1	-177.909463	1	24	22	4	-0.1311
C	1.400007	1	118.255527	1	41.359348	1	26	24	25	-0.0854
C	1.393236	1	119.972414	1	-179.104375	1	27	26	24	-0.1396
C	1.395713	1	120.011327	1	0.502890	1	28	27	26	-0.1053
C	1.395089	1	119.973379	1	0.193048	1	29	28	27	-0.1406
C	1.395104	1	120.330278	1	-0.465768	1	30	29	28	-0.0874
H	1.101391	1	120.513217	1	-178.623376	1	27	28	29	0.1477
H	1.099927	1	120.118829	1	-179.416336	1	28	29	30	0.1386
H	1.100197	1	120.018002	1	179.905863	1	29	30	31	0.1364
H	1.100221	1	119.677281	1	-179.677368	1	30	31	26	0.1389
H	1.101405	1	120.499525	1	-178.201534	1	31	26	27	0.1530
N	1.371070	1	116.793129	1	100.035124	1	6	5	4	-0.2456
H	1.010433	1	109.912659	1	-173.714197	1	37	6	5	0.2239
C	1.421946	1	126.909110	1	-33.605359	1	37	6	5	0.3134
O	1.239923	1	123.701940	1	15.858444	1	39	37	6	-0.3193
C	1.494447	1	113.940736	1	-171.042938	1	39	37	6	-0.1169
C	1.397185	1	120.273898	1	102.357613	1	41	39	40	-0.0981
C	1.394501	1	119.700518	1	-178.192518	1	42	41	39	-0.1410
C	1.395066	1	120.109118	1	-0.398294	1	43	42	41	-0.1170
C	1.395072	1	120.003972	1	-0.052868	1	44	43	42	-0.1393
C	1.394152	1	120.251311	1	0.173174	1	45	44	43	-0.0810
H	1.100261	1	120.271521	1	179.935007	1	42	43	44	0.1405
H	1.099621	1	120.073295	1	179.882065	1	43	44	45	0.1324
H	1.099794	1	120.011754	1	-179.853532	1	44	45	46	0.1305
H	1.099809	1	119.708808	1	-179.821485	1	45	46	41	0.1336
H	1.102326	1	119.594165	1	178.546765	1	46	41	42	0.1597
H	1.130403	1	110.335817	1	161.812660	1	1	6	5	0.1388
H	1.133856	1	102.929463	1	-82.239166	1	1	6	5	0.1212
H	1.130562	1	110.066594	1	172.745566	1	3	2	1	0.1205
H	1.132234	1	104.528690	1	-70.997125	1	3	2	1	0.0861
H	1.130661	1	108.165821	1	-179.035920	1	5	4	3	0.1521
H	1.135279	1	110.588454	1	-59.680174	1	5	4	3	0.0741
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C24 H24 N6 O3

MINDO/3
1,3,5-Tribenazmido-1,3,5-hexahydrotriazine monohydrate

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

```
HEAT OF FORMATION        =    -9.060569 KCAL
ELECTRONIC ENERGY        =-44958.858260 EV
CORE-CORE REPULSION      = 39475.575253 EV
GRADIENT NORM            =        3.807906
DIPOLE                   =       11.00390 DEBYE
NO. OF FILLED LEVELS     =       84
IONISATION POTENTIAL     =        8.592674 EV
MOLECULAR WEIGHT         =      444.492
SCF CALCULATIONS         =      182
COMPUTATION TIME         = 79305.14 SECONDS
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        FINAL GEOMETRY OBTAINED                                          CHARGE
     BONDS PRECISE PULAY MINDO T=36000 RESTART
     MINDO/3
     1,3,5-Tribenazmido-1,3,5-hexahydrotriazine monohydrate
C    0.000000  0    0.000000  0    0.000000  0   0  0  0      0.2548
N    1.439497  1    0.000000  0    0.000000  0   1  0  0      0.0615
C    1.439287  1  117.242651  1    0.000000  0   2  1  0      0.2531
N    1.439481  1  103.230964  1   58.486728  1   3  2  1     -0.0597
C    1.439885  1  116.493446  1  -59.733370  1   4  3  2      0.2529
N    1.439784  1  103.673676  1   59.402815  1   5  4  3     -0.0612
N    1.333919  1  116.781007  1  157.093109  1   2  1  6     -0.1266
H    1.046176  1  116.562850  1   73.641943  1   7  2  1      0.0144
C    1.363617  1  128.244400  1 -106.045334  1   7  2  1      0.6183
O    1.213754  1  123.122189  1    0.111717  1   9  7  2     -0.5409
C    1.508405  1  113.734171  1 -179.855081  1   9  7  2     -0.0935
C    1.424710  1  121.873923  1  -87.584602  1  11  9 10      0.0410
C    1.405056  1  122.164230  1  176.302701  1  12 11  9     -0.0034
C    1.405252  1  120.079583  1   -0.065321  1  13 12 11      0.0295
C    1.405239  1  119.434860  1    0.052850  1  14 13 12     -0.0033
C    1.404915  1  120.100951  1   -0.035536  1  15 14 13      0.0408
H    1.107124  1  118.094870  1  179.922433  1  12 13 14     -0.0092
H    1.104869  1  120.241584  1  179.966362  1  13 14 15      0.0017
H    1.105227  1  120.282113  1  179.976166  1  14 15 16     -0.0041
H    1.104886  1  119.668215  1  179.990228  1  15 16 11      0.0016
H    1.107215  1  119.764708  1  179.849019  1  16 11 12     -0.0094
N    1.333763  1  117.021809  1  154.981229  1   4  3  2     -0.1274
H    1.046127  1  116.669041  1   72.812247  1  22  4  3      0.0142
C    1.364069  1  128.104777  1 -107.003706  1  22  4  3      0.6184
O    1.213691  1  123.110216  1    0.046196  1  24 22  4     -0.5403
C    1.508217  1  113.761444  1  180.037180  1  24 22  4      0.0934
C    1.424746  1  121.904134  1   87.948014  1  26 24 25      0.0408
C    1.404908  1  122.155202  1 -176.237440  1  27 26 24     -0.0032
C    1.405158  1  120.093811  1    0.006899  1  28 27 26      0.0295
C    1.405085  1  119.419912  1    0.011968  1  29 28 27     -0.0032
C    1.405106  1  120.112160  1   -0.009216  1  30 29 28      0.0409
H    1.107130  1  118.095844  1 -179.913851  1  27 28 29     -0.0094
H    1.104883  1  120.214271  1  180.034425  1  28 29 30      0.0015
H    1.105214  1  120.290477  1  179.926941  1  29 30 31     -0.0041
H    1.104897  1  119.659963  1  180.029889  1  30 31 26      0.0016
H    1.107111  1  119.756779  1 -179.875343  1  31 26 27     -0.0090
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N	1.334050	1	116.770531	1	156.796063	1	6	5	4	-0.1264
H	1.046114	1	116.621163	1	73.217124	1	37	6	5	0.0146
C	1.363613	1	128.192341	1	-106.655233	1	37	6	5	0.6183
O	1.213793	1	123.138295	1	0.066011	1	39	37	6	-0.5413
C	1.508258	1	113.739835	1	-179.859025	1	39	37	6	-0.0935
C	1.424698	1	121.924697	1	88.294680	1	41	39	40	0.0407
C	1.404987	1	122.137909	1	-176.468962	1	42	41	39	-0.0032
C	1.405208	1	120.143078	1	0.037208	1	43	42	41	0.0294
C	1.405244	1	119.385198	1	0.031984	1	44	43	42	-0.0031
C	1.404715	1	120.119755	1	-0.044411	1	45	44	43	0.0408
H	1.107127	1	118.107601	1	-179.885540	1	42	43	44	-0.0094
H	1.104930	1	120.199208	1	180.071843	1	43	44	45	0.0014
H	1.105167	1	120.310102	1	179.992438	1	44	45	46	-0.0039
H	1.104900	1	119.659629	1	180.016538	1	45	46	41	0.0015
H	1.107086	1	119.748221	1	-179.817266	1	46	41	42	-0.0090
H	1.134746	1	112.094124	1	177.798661	1	1	6	5	-0.0354
H	1.149227	1	114.606882	1	-69.688992	1	1	6	5	-0.1155
H	1.134405	1	112.352862	1	179.830940	1	3	2	1	-0.0357
H	1.148521	1	114.890904	1	-67.378876	1	3	2	1	-0.1129
H	1.134516	1	112.337278	1	-179.252771	1	5	4	3	-0.0358
H	1.148709	1	114.786239	1	-66.595312	1	5	4	3	-0.1137
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF   MNDO   CALCULATION

VERSION   3.00

C24 H24 N6   O3

MNDO
1,3,5-Tribenazmido-1,3,5-hexahydrotriazine monohydrate

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   79.288870 KCAL
ELECTRONIC ENERGY   =-47384.397086 EV
CORE-CORE REPULSION   = 41771.757305 EV
GRADIENT NORM   =   16.986867
DIPOLE   =   3.20595 DEBYE
NO. OF FILLED LEVELS   =   84
IONISATION POTENTIAL   =   9.361125 EV
MOLECULAR WEIGHT   =   444.492
SCF CALCULATIONS   =   150
COMPUTATION TIME   = 94627.86 SECONDS

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FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 SHIFT=30 RESTART
MNDO
1,3,5-Tribenazmido-1,3,5-hexahydrotriazine monohydrate

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.3277
N	1.481359	1	0.000000	0	0.000000	0	1	0	0	-0.3294
C	1.473541	1	116.774271	1	0.000000	0	2	1	0	0.2653
N	1.492041	1	107.908183	1	51.039725	1	3	2	1	-0.2824
C	1.492502	1	112.202441	1	-64.057605	1	4	3	2	0.2920
N	1.476469	1	109.402848	1	56.776512	1	5	4	3	-0.3579
N	1.369657	1	123.450016	1	117.238354	1	2	1	6	-0.2238
H	1.021392	1	107.839109	1	86.589147	1	7	2	1	0.1490
C	1.444334	1	126.301923	1	-46.221027	1	7	2	1	0.3517
O	1.220503	1	123.098516	1	-1.788424	1	9	7	2	-0.2896
C	1.504207	1	112.773604	1	-178.701446	1	9	7	2	-0.1113
C	1.412762	1	120.314287	1	-93.228897	1	11	9	10	0.0026
C	1.407193	1	120.353602	1	178.458310	1	12	11	9	-0.0711
C	1.405601	1	120.141792	1	-0.028216	1	13	12	11	-0.0374
C	1.406263	1	119.844052	1	-0.172704	1	14	13	12	-0.0707
C	1.405131	1	120.176477	1	0.119723	1	15	14	13	-0.0257
H	1.091419	1	119.152730	1	179.594008	1	12	13	14	0.0794
H	1.090322	1	120.067910	1	179.773079	1	13	14	15	0.0654
H	1.090455	1	120.038080	1	179.947618	1	14	15	16	0.0618
H	1.090393	1	119.816320	1	179.901957	1	15	16	11	0.0628
H	1.091283	1	120.592720	1	179.394376	1	16	11	12	0.0596
N	1.375983	1	117.367398	1	166.741110	1	4	3	2	-0.2365
H	1.021017	1	114.072878	1	33.038528	1	22	4	3	0.1246
C	1.448738	1	116.774621	1	-97.323802	1	22	4	3	0.3596
O	1.219857	1	122.881278	1	0.012635	1	24	22	4	-0.2719
C	1.504425	1	112.785858	1	-176.155206	1	24	22	4	-0.1148
C	1.414021	1	120.560590	1	84.829954	1	26	24	25	-0.0257
C	1.404801	1	120.409641	1	-178.750027	1	27	26	24	-0.0689
C	1.406300	1	120.137578	1	0.137284	1	28	27	26	-0.0372
C	1.404964	1	119.850572	1	0.114279	1	29	28	27	-0.0704
C	1.406947	1	120.216886	1	-0.094667	1	30	29	28	-0.0010
H	1.091245	1	119.116169	1	-179.570930	1	27	28	29	0.0605
H	1.090419	1	120.009804	1	-179.800249	1	28	29	30	0.0637
H	1.090497	1	120.118425	1	180.021892	1	29	30	31	0.0627
H	1.090465	1	119.756504	1	180.044820	1	30	31	26	0.0653
H	1.091329	1	120.568619	1	-179.459360	1	31	26	27	0.0739
N	1.370391	1	122.270845	1	117.563569	1	6	5	4	-0.2112
H	1.022780	1	107.645453	1	86.641436	1	37	6	5	0.1404
C	1.447873	1	125.719796	1	-43.898554	1	37	6	5	0.3428
O	1.219549	1	123.566235	1	-4.578376	1	39	37	6	-0.2731
C	1.505305	1	112.447593	1	178.679321	1	39	37	6	-0.1093
C	1.413940	1	120.518468	1	85.664886	1	41	39	40	-0.0260
C	1.405172	1	120.414077	1	-178.632446	1	42	41	39	-0.0697
C	1.406201	1	120.128762	1	0.166811	1	43	42	41	-0.0384
C	1.404547	1	119.823280	1	0.083967	1	44	43	42	-0.0717
C	1.407360	1	120.239287	1	-0.133776	1	45	44	43	0.0007
H	1.091278	1	118.993865	1	-179.536892	1	42	43	44	0.0601
H	1.090368	1	120.025183	1	-179.792015	1	43	44	45	0.0628
H	1.090454	1	120.122605	1	179.996123	1	44	45	46	0.0616

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H    1.090427  1  119.741875  1 -179.797650  1  45 46 41       0.0641
H    1.091126  1  120.516505  1 -179.424349  1  46 41 42       0.0753
H    1.117528  1  112.182041  1  155.075488  1   1  6  5       0.0355
H    1.130369  1  105.863304  1  -89.501584  1   1  6  5       0.0037
H    1.118725  1  111.640243  1  172.664619  1   3  2  1       0.0373
H    1.126738  1  107.576335  1  -70.986125  1   3  2  1      -0.0079
H    1.116939  1  110.506798  1 -178.830755  1   5  4  3       0.0390
H    1.129489  1  112.047127  1  -61.057452  1   5  4  3      -0.0181
0    0.000000  0    0.000000  0    0.000000  0   0  0  0
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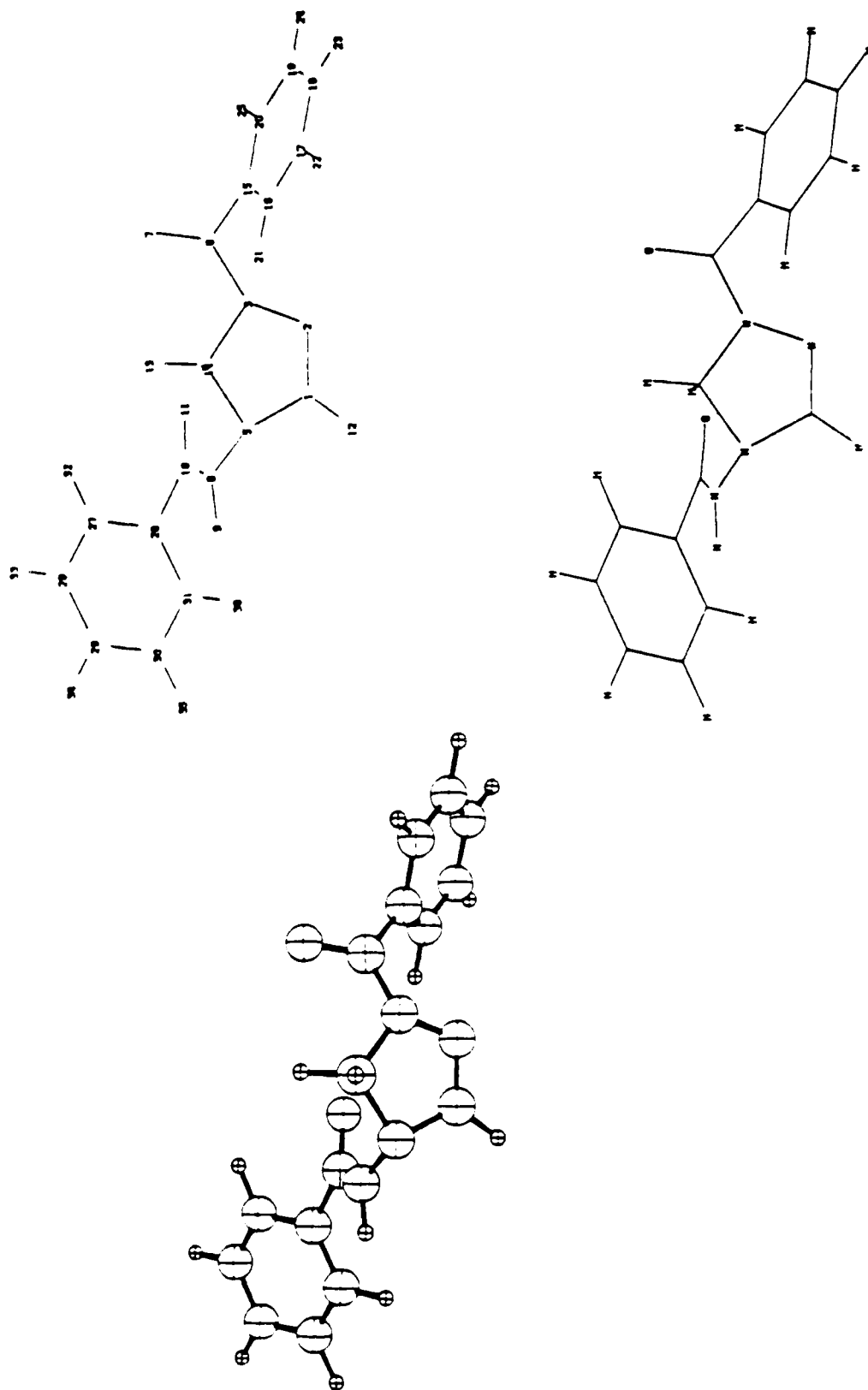
Figure A 16. 1-Benzoyl-4-benzamido-Δ^2-1,2,4-triazoline [Ref. A 12].

VERSION   3.10

C16 H14 N4   O2

23-FEB-87

AM1
1-Benzoyl-4-benzamido-D2-1,2,4-triazine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	92.057401 KCAL
ELECTRONIC ENERGY	=	-24538.460525 EV
CORE-CORE REPULSION	=	20833.058290 EV
GRADIENT NORM	=	3.115747
DIPOLE	=	4.82712 DEBYE
NO. OF FILLED LEVELS	=	55
IONISATION POTENTIAL	=	9.379683 EV
MOLECULAR WEIGHT	=	294.312
SCF CALCULATIONS	=	12
COMPUTATION TIME	=	5701.81 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000
AM1
1-Benzoyl-4-benzamido-D2-1,2,4-triazine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1448
N	1.318245	1	0.000000	0	0.000000	0	1	0	0	-0.0036
N	1.362891	1	109.098078	1	0.000000	0	2	1	0	-0.2588
C	1.498712	1	109.613635	1	0.343142	1	3	2	1	-0.0271
N	1.519164	1	105.631040	1	-1.350420	1	4	3	2	-0.0753
C	1.421949	1	118.578502	1	146.784475	1	3	4	5	0.3650
O	1.240794	1	117.756178	1	21.290637	1	6	3	4	-0.3213
N	1.361815	1	115.988789	1	-123.879583	1	5	4	3	-0.3279
H	1.000684	1	111.616540	1	-130.934694	1	8	5	4	0.2525
C	1.402456	1	126.955274	1	67.343571	1	8	5	4	0.3308
O	1.245191	1	121.021632	1	-170.682262	1	10	8	9	-0.3487
H	1.096945	1	124.261433	1	-175.819762	1	1	2	3	0.2051
H	1.124679	1	111.432513	1	-126.727042	1	4	3	2	0.1362
H	1.125013	1	107.977629	1	111.338721	1	4	3	2	0.1385
C	1.484226	1	118.858126	1	-19.501822	1	6	3	2	-0.1042
C	1.398156	1	120.593381	1	-118.486794	1	15	6	7	-0.0784
C	1.394915	1	119.569948	1	178.061264	1	16	15	6	-0.1384
C	1.394694	1	120.164219	1	0.344614	1	17	16	15	-0.1097
C	1.395281	1	120.122894	1	-0.457270	1	18	17	16	-0.1396
C	1.393923	1	120.092507	1	0.083933	1	19	18	17	-0.0834
H	1.101351	1	120.072055	1	179.891601	1	16	17	18	0.1518
H	1.099803	1	120.116661	1	179.702311	1	17	18	19	0.1361
H	1.100098	1	119.916346	1	179.954665	1	18	19	20	0.1326

											CHARGE
H	1.099752	1	119.804596	1	-179.738703	1	19	20	15		0.1356
H	1.100507	1	119.818725	1	179.190787	1	20	15	16		0.1444
C	1.487828	1	116.390076	1	172.996749	1	10	8	5		-0.1225
C	1.400361	1	118.098966	1	-38.944157	1	26	10	11		-0.0740
C	1.393978	1	119.820218	1	179.308156	1	27	26	10		-0.1349
C	1.395065	1	120.092436	1	-0.342058	1	28	27	26		-0.1040
C	1.395136	1	120.056713	1	-0.248237	1	29	28	27		-0.1358
C	1.394461	1	120.172960	1	0.515861	1	30	29	28		-0.1046
H	1.101913	1	120.720698	1	179.028767	1	27	28	29		0.1568
H	1.100266	1	120.111531	1	179.615070	1	28	29	30		0.1420
H	1.100426	1	119.939727	1	-179.782197	1	29	30	31		0.1384
H	1.100111	1	119.796418	1	179.749651	1	30	31	26		0.1389
H	1.100249	1	120.847083	1	178.346568	1	31	26	27		0.1323
0	0.000000	0	0.000000	0	0.000000	0	0	0	0		

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C16 H14 N4 02

30-MAR-86

MINDO/3
1-Benzoyl-4-benzamido-D2-1,2,4-triazine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-17.440970 KCAL
ELECTRONIC ENERGY	=	-23255.017818 EV
CORE-CORE REPULSION	=	19628.530071 EV
DIPOLE	=	5.96309 DEBYE
NO. OF FILLED LEVELS	=	55
IONISATION POTENTIAL	=	7.801098 EV
MOLECULAR WEIGHT	=	294.312
SCF CALCULATIONS	=	129
COMPUTATION TIME	=	171330.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000 RESTART
MINDO/3
1 Benzoyl-4-benzamido-D2-1,2,4-triazine

											CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0		0.1641
N	1.291226	1	0.000000	0	0.000000	0	1	0	0		-0.1417
N	1.347817	1	108.904283	1	0.000000	0	2	1	0		-0.1261
C	1.441817	1	111.805477	1	-0.282264	1	3	2	1		0.2397

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N	1.440378	1	99.700538	1	-1.797232	1	4	3	2	-0.0451
C	1.376201	1	127.679891	1	179.407541	1	3	4	5	0.6132
O	1.217633	1	120.400415	1	0.851073	1	6	3	4	-0.5649
N	1.323457	1	123.500506	1	171.369114	1	5	4	3	-0.1291
H	1.043235	1	114.982686	1	-74.422834	1	8	5	4	0.0292
C	1.361765	1	128.775811	1	104.744823	1	8	5	4	0.6166
O	1.216741	1	122.134231	1	-178.713332	1	10	8	9	-0.5615
H	1.113454	1	125.466949	1	-178.875244	1	1	2	3	0.0326
H	1.135386	1	114.554324	1	-122.340644	1	4	3	2	-0.0419
H	1.138909	1	114.945782	1	120.563193	1	4	3	2	-0.0701
C	1.507293	1	118.576664	1	2.401788	1	6	3	2	-0.0836
C	1.424726	1	121.935512	1	-87.901735	1	15	6	7	0.0392
C	1.405299	1	122.249992	1	175.982586	1	16	15	6	-0.0025
C	1.405163	1	120.087670	1	-0.194974	1	17	16	15	0.0262
C	1.405142	1	119.337797	1	-0.086247	1	18	17	16	-0.0029
C	1.404953	1	120.189991	1	0.076449	1	19	18	17	0.0379
H	1.107252	1	117.934370	1	179.587626	1	16	17	18	-0.0088
H	1.104946	1	120.224179	1	179.779244	1	17	18	19	0.0005
H	1.105243	1	120.297888	1	179.972553	1	18	19	20	-0.0053
H	1.105132	1	119.638442	1	-179.922566	1	19	20	15	-0.0011
H	1.107441	1	119.873939	1	179.318702	1	20	15	16	-0.0122
C	1.506368	1	114.464450	1	-178.581106	1	10	8	5	-0.0965
C	1.424803	1	121.790417	1	-87.953805	1	26	10	11	0.0422
C	1.405024	1	122.067169	1	176.646766	1	27	26	10	-0.0024
C	1.405183	1	120.183589	1	-0.023324	1	28	27	26	0.0308
C	1.405349	1	119.381488	1	-0.009750	1	29	28	27	-0.0030
C	1.404938	1	120.092306	1	0.004545	1	30	29	28	0.0402
H	1.106873	1	118.190380	1	179.895141	1	27	28	29	-0.0063
H	1.104791	1	120.204643	1	179.940110	1	28	29	30	0.0039
H	1.105047	1	120.289483	1	179.989400	1	29	30	31	-0.0020
H	1.104817	1	119.640976	1	179.999194	1	30	31	26	0.0026
H	1.107341	1	119.701104	1	179.869573	1	31	26	27	-0.0123
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C16 H14 N4 O2

2-APR-86

MNDO
1-Benzoyl-4-benzamido-D2-1,2,4-triazine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   42.350004 KCAL
ELECTRONIC ENERGY   =-23713.746192 EV
CORE-CORE REPULSION   = 19999.861800 EV
DIPOLE   =   5.32335 DEBYE
NO. OF FILLED LEVELS   =   55
IONISATION POTENTIAL   =   9.351279 EV
MOLECULAR WEIGHT   =   294.312
SCF CALCULATIONS   =   21
COMPUTATION TIME   =185692.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 RESTART
MNDO
1-Benzoyl-4-benzamido-D2-1,2,4-triazine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0059
N	1.313426	1	0.000000	0	0.000000	0	1	0	0	-0.0673
N	1.350957	1	108.992122	1	0.000000	0	2	1	0	-0.3734
C	1.490886	1	111.919576	1	1.263727	1	3	2	1	0.2736
N	1.500226	1	101.444900	1	0.581471	1	4	3	2	-0.2086
C	1.428360	1	126.982788	1	169.640798	1	3	4	5	0.4372
O	1.225513	1	117.416728	1	4.042906	1	6	3	4	-0.3345
N	1.377878	1	113.841911	1	-131.882672	1	5	4	3	-0.2447
H	1.018732	1	113.824746	1	108.607268	1	8	5	4	0.1425
C	1.447672	1	115.765243	1	-120.179059	1	8	5	4	0.3640
O	1.221013	1	121.157749	1	154.576577	1	10	8	9	-0.2788
H	1.087183	1	124.987510	1	-177.593599	1	1	2	3	0.1381
H	1.116552	1	112.575336	1	-122.855621	1	4	3	2	0.0382
H	1.118704	1	110.471736	1	115.201953	1	4	3	2	0.0493
C	1.499005	1	118.011626	1	-9.416309	1	6	3	2	-0.0921
C	1.413640	1	120.339998	1	-86.464029	1	15	6	7	-0.0104
C	1.405752	1	120.294343	1	178.331311	1	16	15	6	-0.0692
C	1.405963	1	120.182754	1	0.018919	1	17	16	15	-0.0351
C	1.405549	1	119.830437	1	-0.096025	1	18	17	16	-0.0685
C	1.406286	1	120.222736	1	0.062356	1	19	18	17	-0.0035
H	1.091128	1	119.140897	1	179.893503	1	16	17	18	0.0626
H	1.090378	1	120.022697	1	179.891553	1	17	18	19	0.0638
H	1.090451	1	120.093087	1	180.032402	1	18	19	20	0.0626
H	1.090431	1	119.755596	1	180.018757	1	19	20	15	0.0650
H	1.091186	1	120.584405	1	179.787203	1	20	15	16	0.0676
C	1.502742	1	114.118613	1	-162.858514	1	10	8	5	-0.1308
C	1.413912	1	120.253678	1	-84.563834	1	26	10	11	-0.0194
C	1.405450	1	120.362460	1	178.618034	1	27	26	10	-0.0672
C	1.406318	1	120.136935	1	-0.131297	1	28	27	26	-0.0316
C	1.405462	1	119.845245	1	-0.081058	1	29	28	27	-0.0681
C	1.406600	1	120.207421	1	0.057545	1	30	29	28	-0.0039
H	1.091300	1	119.105215	1	179.515025	1	27	28	29	0.0640
H	1.090423	1	120.033701	1	179.742964	1	28	29	30	0.0671
H	1.090542	1	120.100195	1	179.920145	1	29	30	31	0.0659
H	1.090494	1	119.761049	1	180.024858	1	30	31	26	0.0682
H	1.091291	1	120.549872	1	179.395386	1	31	26	27	0.0714
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

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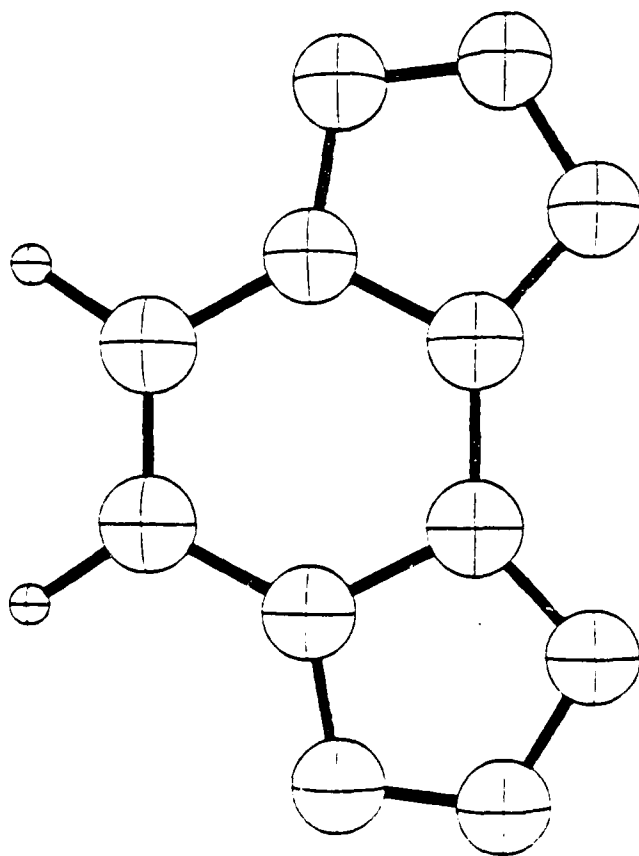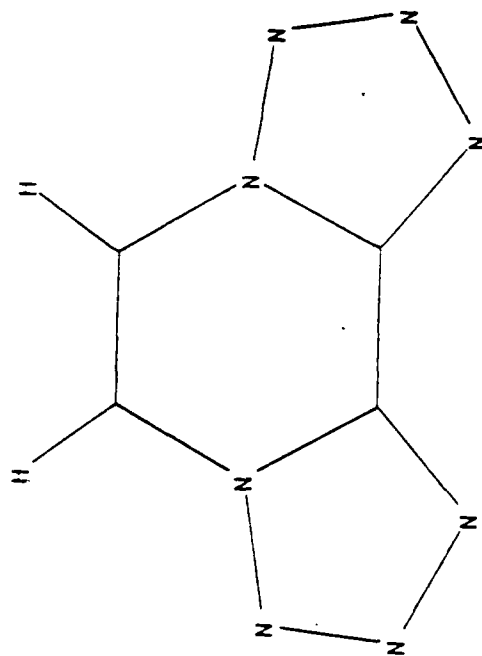
Figure A-17. Bis-tetrazolo[1,5-a:1',5'-c]pyrazine [Ref. A-12].

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VERSION   3.00

C4   H2   N8

AM1
bis-Tetrazolo[1,5-a:1',5'-c]pyrazine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	243.702444 KCAL
ELECTRONIC ENERGY	=	-9767.968668 EV
CORE-CORE REPULSION	=	7579.858033 EV
DIPOLE	=	5.16590 DEBYE
NO. OF FILLED LEVELS	=	29
IONISATION POTENTIAL	=	9.470872 EV
MOLECULAR WEIGHT	=	162.113
SCF CALCULATIONS	=	303
COMPUTATION TIME	=	2151.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 SHIFT=50
AM1
bis-Tetrazolo[1,5-a:1',5'-c]pyrazine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0800
C	1.461464	1	0.000000	0	0.000000	0	1	0	0	0.1349
N	1.342412	1	120.539791	1	0.000000	0	2	1	0	-0.1905
C	1.371155	1	118.580108	1	-0.085121	1	3	2	1	-0.0808
C	1.385613	1	125.439762	1	0.012815	1	4	3	2	-0.0904
N	1.389117	1	117.574741	1	0.026525	1	5	4	3	-0.0700
N	1.413885	1	114.025443	1	-179.923152	1	2	1	6	-0.1859
N	1.275045	1	120.818874	1	-179.552823	1	7	2	1	0.2328
N	1.127879	1	169.452433	1	179.632166	1	8	7	2	0.0563
N	1.348514	1	133.204812	1	179.988448	1	6	5	4	-0.0252
N	1.289928	1	106.929507	1	180.020811	1	10	6	5	-0.0317
N	1.322589	1	114.616713	1	-0.003198	1	11	10	6	-0.0530
H	1.105579	1	114.365177	1	180.023392	1	4	3	2	0.1875
H	1.101223	1	124.567616	1	180.027701	1	5	4	3	0.1959
0	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION   3.00

C4 H2 N8

MINDO/3
bis-Tetrazolo[1,5-a:1',5'-c]pyrazine

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

          HEAT OF FORMATION   =   -44.872757 KCAL
          ELECTRONIC ENERGY   = -9551.330925 EV
          CORE-CORE REPULSION   = 7473.054704 EV
          DIPOLE   =   2.52051 DEBYE
          NO. OF FILLED LEVELS   =   29
          IONISATION POTENTIAL   =   7.586209 EV
          MOLECULAR WEIGHT   =   162.113
          SCF CALCULATIONS   =   272
          COMPUTATION TIME   =   1366.39 SECONDS

          FINAL GEOMETRY OBTAINED   CHARGE
          BONDS PRECISE PULAY MINDO T=36000 SHIFT=50
          MINDO/3
          bis-Tetrazolo[1,5-a:1',5'-c]pyrazine

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0398
C	1.455615	1	0.000000	0	0.000000	0	1	0	0	0.3335
N	1.309350	1	121.874145	1	0.000000	0	2	1	0	-0.2771
C	1.368107	1	120.041605	1	-0.031703	1	3	2	1	0.1115
C	1.371458	1	123.190005	1	-0.000267	1	4	3	2	-0.1005
N	1.389432	1	117.564239	1	-0.007735	1	5	4	3	0.1791
N	1.365305	1	117.011135	1	-179.917828	1	2	1	6	-0.3973
N	1.188838	1	132.135421	1	-178.851176	1	7	2	1	0.6357
N	1.103415	1	168.722242	1	179.567873	1	8	7	2	-0.2757
N	1.296523	1	130.374773	1	180.012320	1	6	5	4	-0.1064
N	1.235825	1	106.636117	1	180.003134	1	10	6	5	0.0411
N	1.263865	1	115.645598	1	0.022685	1	11	10	6	-0.1188
H	1.113129	1	115.869594	1	180.006430	1	4	3	2	-0.0044
H	1.111187	1	122.833757	1	180.014391	1	5	4	3	0.0190
0	0.000000	0	0.000000	0	0.000000	0	0	0	0	

                    SUMMARY OF MNDO   CALCULATION

                                              VERSION 3.00

C4 H2 N8

MNDO
bis-Tetrazolo[1,5-a:1',5'-c]pyrazine

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	136.018018 KCAL
ELECTRONIC ENERGY	=	-10152.241832 EV
CORE-CORE REPULSION	=	7958.315040 EV
GRADIENT NORM	=	2.798138
DIPOLE	=	6.05487 DEBYE
NO. OF FILLED LEVELS	=	29
IONISATION POTENTIAL	=	10.749354 EV
MOLECULAR WEIGHT	=	162.113
SCF CALCULATIONS	=	232
COMPUTATION TIME	=	1550.67 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 SHIFT=50
MNDO
bis-Tetrazolo[1,5-a:1',5'-c]pyrazine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0832
C	1.432719	1	0.000000	0	0.000000	0	1	0	0	0.0838
N	1.422433	1	116.923590	1	0.000000	0	2	1	0	-0.1797
C	1.419306	1	124.436195	1	0.018840	1	3	2	1	0.0637
C	1.368274	1	118.670379	1	-0.019345	1	4	3	2	0.0645
N	1.419688	1	118.392771	1	0.006484	1	5	4	3	-0.1794
N	1.349205	1	137.606254	1	179.995845	1	2	1	6	-0.0821
N	1.327848	1	106.558080	1	179.989763	1	7	2	1	-0.0258
N	1.275459	1	113.596318	1	-0.015871	1	8	7	2	0.0057
N	1.344175	1	128.405559	1	179.989107	1	6	5	4	0.0052
N	1.275272	1	107.278896	1	180.007209	1	10	6	5	-0.0257
N	1.327759	1	113.581003	1	-0.003904	1	11	10	6	-0.0823
H	1.091740	1	117.144874	1	179.917635	1	4	3	2	0.1342
H	1.091470	1	124.337433	1	180.048977	1	5	4	3	0.1348
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

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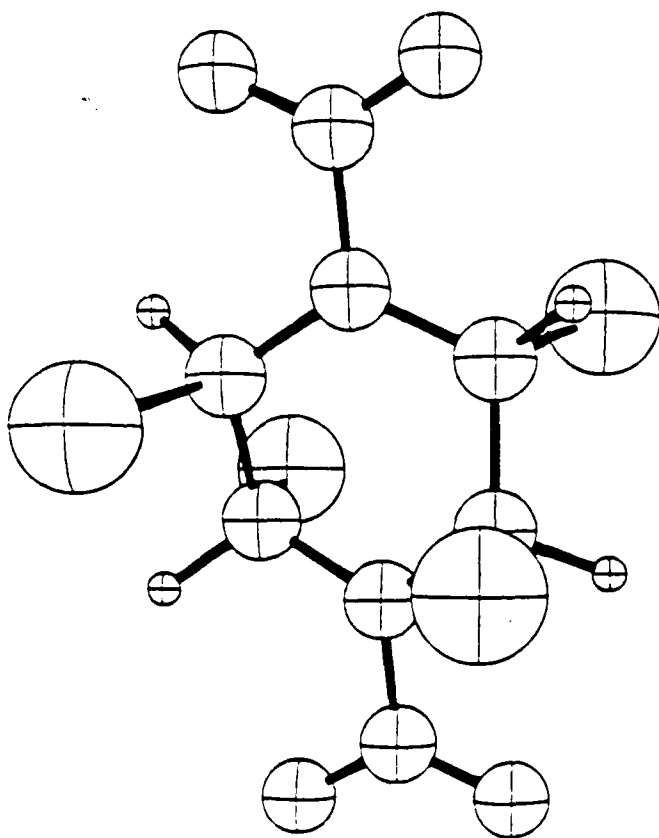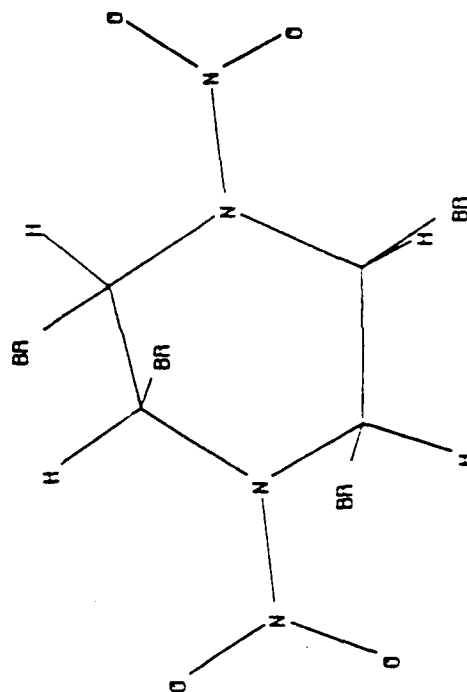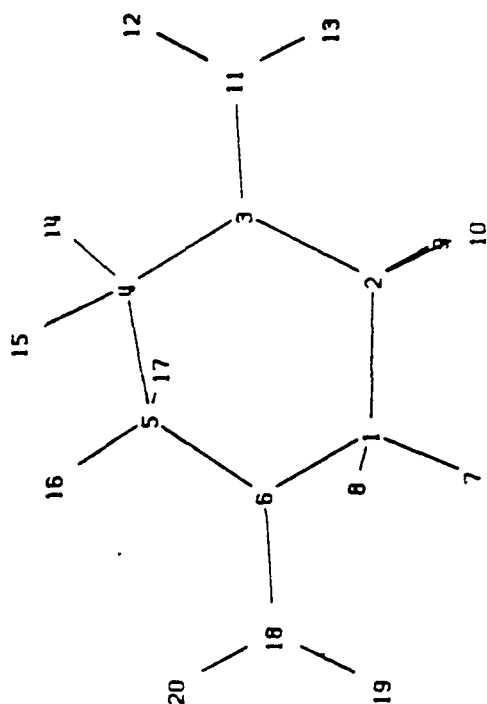
Figure A-18. 1,4-Dinitro-2,3,5,6-tetrabromo-2,3,5,6-piperazine [Ref. A-12].

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C4   H4   N4   O4 Br4

AM1
1,4-Dinitro-2,3,5,6-tetrabromo-2,3,5,6-piperazine

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	110.302522 KCAL
ELECTRONIC ENERGY	=	-20835.846230 EV
CORE-CORE REPULSION	=	16777.778757 EV
DIPOLE	=	0.02671 DEBYE
NO. OF FILLED LEVELS	=	46
IONISATION POTENTIAL	=	11.481969 EV
MOLECULAR WEIGHT	=	491.716
SCF CALCULATIONS	=	746
COMPUTATION TIME	=	11615.14 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 SHIFT=30
AM1
1,4-Dinitro-2,3,5,6-tetrabromo-2,3,5,6-piperazine

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0528
C	1.525704	1	0.000000	0	0.000000	0	1	0	0	0.0528
N	1.432635	1	115.783203	1	0.000000	0	2	1	0	-0.3490
C	1.432558	1	120.545813	1	-18.396639	1	3	2	1	0.0527
C	1.525153	1	116.114398	1	-16.386710	1	4	3	2	0.0529
N	1.432850	1	116.014199	1	34.805534	1	5	4	3	-0.3492
H	1.128257	1	110.432514	1	165.401000	1	1	2	3	0.2017
Br	1.979833	1	105.067715	1	-86.258052	1	1	2	3	-0.1190
H	1.128219	1	112.214054	1	-146.408816	1	2	3	4	0.2017
Br	1.979326	1	110.937491	1	101.223166	1	2	3	4	-0.1190
N	1.417211	1	119.721696	1	162.875850	1	3	2	1	0.6719
O	1.194431	1	117.042167	1	167.560760	1	11	3	2	-0.2971
O	1.194474	1	117.046248	1	-12.538744	1	11	3	2	-0.2969
H	1.128358	1	112.283754	1	-144.772695	1	4	3	2	0.2017
Br	1.980443	1	110.694709	1	103.013976	1	4	3	2	-0.1187
H	1.128370	1	110.369044	1	163.940982	1	5	4	3	0.2017
Br	1.980007	1	105.011868	1	-87.780080	1	5	4	3	-0.1188
N	1.417071	1	119.752185	1	162.566511	1	6	5	4	0.6719
O	1.194443	1	117.049853	1	168.413375	1	18	6	5	-0.2972
O	1.194411	1	117.090290	1	-11.491718	1	18	6	5	-0.2970
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C4 H4 N4 O4 Br4

    MNDO
    1,4-Dinitro-2,3,5,6-tetrabromo-2,3,5,6-piperazine

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	94.227150 KCAL
ELECTRONIC ENERGY	=	-20857.468265 EV
CORE-CORE REPULSION	=	16790.155258 EV
GRADIENT NORM	=	2.638884
DIPOLE	=	0.11308 DEBYE
NO. OF FILLED LEVELS	=	46
IONISATION POTENTIAL	=	11.902230 EV
MOLECULAR WEIGHT	=	491.716
SCF CALCULATIONS	=	786
COMPUTATION TIME	=	12229.28 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 SHIFT=25
MNDO
1,4-Dinitro-2,3,5,6-tetrabromo-2,3,5,6-piperazine

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.1660
C	1.551186	1	0.000000	0	0.000000	0	1	0	0	0.1658
N	1.462868	1	114.130101	1	0.000000	0	2	1	0	-0.4102
C	1.461972	1	121.428779	1	-16.546379	1	3	2	1	0.1646
C	1.550837	1	113.321292	1	-25.033505	1	4	3	2	0.1678
N	1.461846	1	113.398588	1	43.873224	1	5	4	3	-0.4134
H	1.118512	1	106.878261	1	164.830291	1	1	2	3	0.1034
Br	1.906688	1	110.203994	1	-83.821328	1	1	2	3	-0.0863
H	1.118665	1	112.661953	1	-138.864733	1	2	3	4	0.1030
Br	1.906192	1	109.061385	1	106.756135	1	2	3	4	-0.0818
N	1.414013	1	119.302294	1	158.688662	1	3	2	1	0.6200
O	1.204271	1	117.688912	1	156.493879	1	11	3	2	-0.2883
O	1.204393	1	118.039480	1	-22.814918	1	11	3	2	-0.2910
H	1.118629	1	112.199165	1	-146.221071	1	4	3	2	0.1040
Br	1.906362	1	110.395883	1	99.320256	1	4	3	2	-0.0861
H	1.118471	1	107.116496	1	168.487773	1	5	4	3	0.1028
Br	1.905889	1	110.168460	1	-79.699780	1	5	4	3	-0.0843
N	1.414510	1	119.117982	1	160.064625	1	6	5	4	0.6202
O	1.203940	1	117.920753	1	151.039800	1	18	6	5	-0.2883
O	1.203961	1	117.739326	1	-29.263808	1	18	6	5	-0.2880
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	
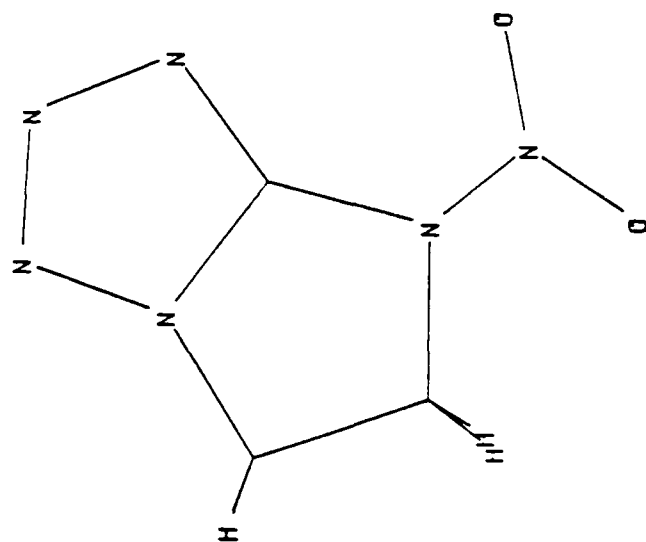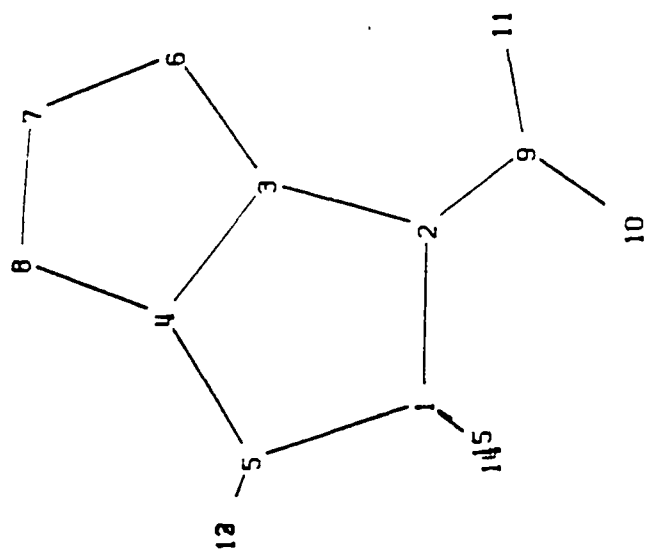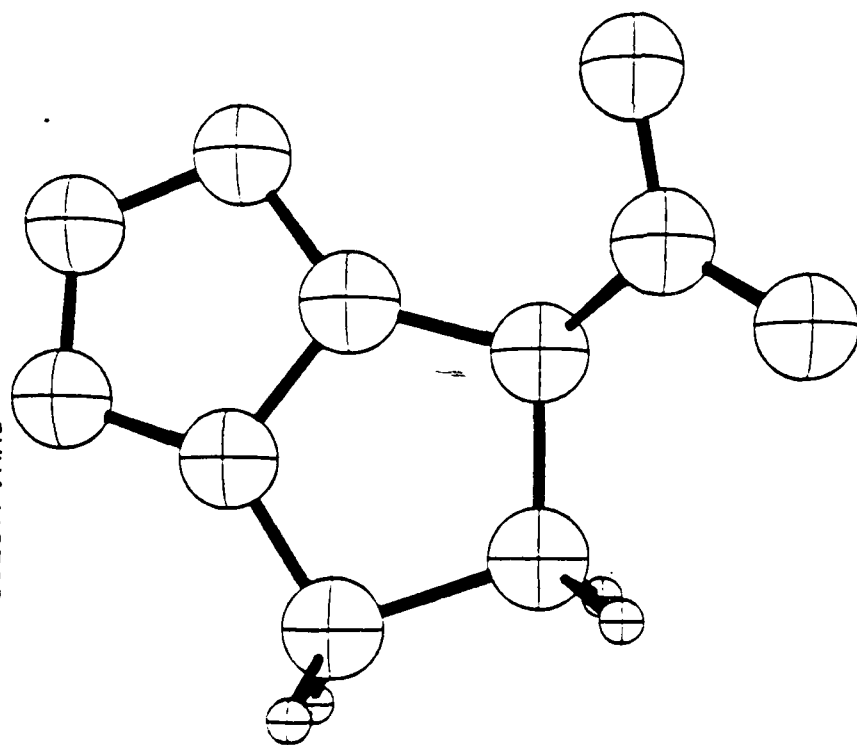
Figure A-19. 7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]-tetrazole [Ref. A-12].

C3   H4   N6   O2

AM1
7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	177.031201 KCAL
ELECTRONIC ENERGY	=-10300.824668 EV
CORE-CORE REPULSION	=	7987.988810 EV
DIPOLE	=	6.50550 DEBYE
NO. OF FILLED LEVELS	=	29
IONISATION POTENTIAL	=	10.969069 EV
MOLECULAR WEIGHT	=	156.104
SCF CALCULATIONS	=	686
COMPUTATION TIME	=	4010.69 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000
AM1
7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1014
N	1.502041	1	0.000000	0	0.000000	0	1	0	0	-0.1510
C	1.429239	1	104.677348	1	0.000000	0	2	1	0	-0.0429
N	1.441723	1	112.723597	1	2.178628	1	3	2	1	-0.2036
C	1.450940	1	110.476110	1	-2.599641	1	4	3	2	-0.0198
N	1.364568	1	106.034342	1	173.529097	1	3	4	5	-0.0103
N	1.340776	1	104.492660	1	173.208843	1	6	3	2	-0.0617
N	1.288355	1	115.365583	1	-0.601901	1	7	6	3	0.0456
N	1.436303	1	116.867254	1	56.022897	1	2	3	6	0.6025
O	1.200098	1	116.465221	1	150.056619	1	9	2	3	-0.3389
O	1.192438	1	118.397134	1	-35.319504	1	9	2	3	-0.2762
H	1.122206	1	111.346805	1	49.557791	1	5	4	8	0.1343
H	1.122096	1	110.217860	1	-72.476937	1	5	4	8	0.1306
H	1.122904	1	110.367512	1	123.622001	1	1	5	4	0.1467
H	1.122778	1	110.302874	1	-115.447470	1	1	5	4	0.1462
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

C3 H4 N6 O2

MINDO/3
7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	-58.508091 KCAL
ELECTRONIC ENERGY	=	-10103.487037 EV
CORE-CORE REPULSION	=	7887.486017 EV
DIPOLE	=	4.89528 DEBYE
NO. OF FILLED LEVELS	=	29
IONISATION POTENTIAL	=	9.034248 EV
MOLECULAR WEIGHT	=	156.104
SCF CALCULATIONS	=	357
COMPUTATION TIME	=	1081.23 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000
MINDO/3
7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.1669
N	1.477124	1	0.000000	0	0.000000	0	1	0	0	-0.2579
C	1.405103	1	108.543821	1	0.000000	0	2	1	0	0.1762
N	1.391680	1	108.935010	1	-0.338845	1	3	2	1	-0.0209
C	1.440984	1	112.577729	1	0.402663	1	4	3	2	0.1031
N	1.328428	1	105.646989	1	-179.746038	1	3	4	5	-0.0981
N	1.287990	1	103.714066	1	179.675505	1	6	3	2	0.0256
N	1.224761	1	117.326935	1	0.079501	1	7	6	3	-0.0050
N	1.304991	1	124.194744	1	0.039096	1	2	3	6	1.1796
O	1.230522	1	113.829440	1	-0.131790	1	9	2	3	-0.5859
O	1.230432	1	115.140758	1	179.879703	1	9	2	3	-0.5942
H	1.125199	1	114.182277	1	58.122210	1	5	4	8	-0.0249
H	1.125236	1	114.159660	1	-58.149320	1	5	4	8	-0.0250
H	1.125133	1	111.408747	1	123.153549	1	1	5	4	-0.0198
H	1.125120	1	111.413767	1	-123.002671	1	1	5	4	-0.0198
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

C3   H4   N6   O2

MNDO
7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   99.180489 KCAL
ELECTRONIC ENERGY   =-10311.748714 EV
CORE-CORE REPULSION   = 7989.864444 EV
DIPOLE   =   ·6.44808 DEBYE
NO. OF FILLED LEVELS   =   29
IONISATION POTENTIAL   =   11.109256 EV
MOLECULAR WEIGHT   =   156.104
SCF CALCULATIONS   =   393
COMPUTATION TIME   =   1879.38 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 SHIFT=25
MNDO
7-Nitro-5,6-dihydro-7H-imidazolo[1,2-d]tetrazole

|										
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.1167
N	1.515062	1	0.000000	0	0.000000	0	1	0	0	-0.2625
C	1.410612	1	106.948819	1	0.000000	0	2	1	0	0.1138
N	1.404133	1	110.536206	1	3.138381	1	3	2	1	-0.2694
C	1.466961	1	113.535262	1	0.325613	1	4	3	2	0.1746
N	1.347118	1	106.896020	1	-174.123519	1	3	4	5	-0.0858
N	1.336484	1	104.804048	1	-170.855313	1	6	3	2	-0.0437
N	1.276854	1	114.364326	1	0.667301	1	7	6	3	0.0279
N	1.415311	1	120.255298	1	-43.702150	1	2	3	6	0.5868
O	1.202729	1	118.880798	1	6.906705	1	9	2	3	-0.2728
O	1.206302	1	116.068906	1	-177.574165	1	9	2	3	-0.3023
H	1.113302	1	111.047894	1	67.697866	1	5	4	8	0.0506
H	1.113353	1	111.719449	1	-52.966056	1	5	4	8	0.0537
H	1.114186	1	111.177520	1	122.384278	1	1	5	4	0.0635
H	1.113578	1	110.191380	1	-117.798714	1	1	5	4	0.0489
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

IETNFCD.ARC
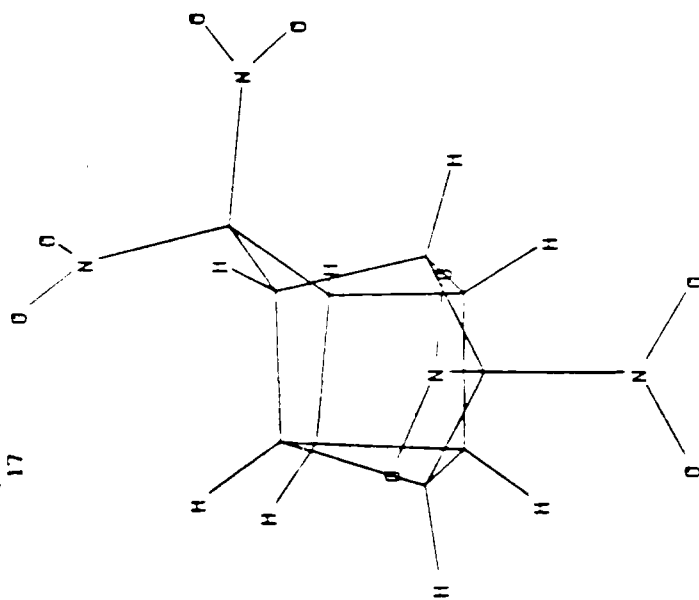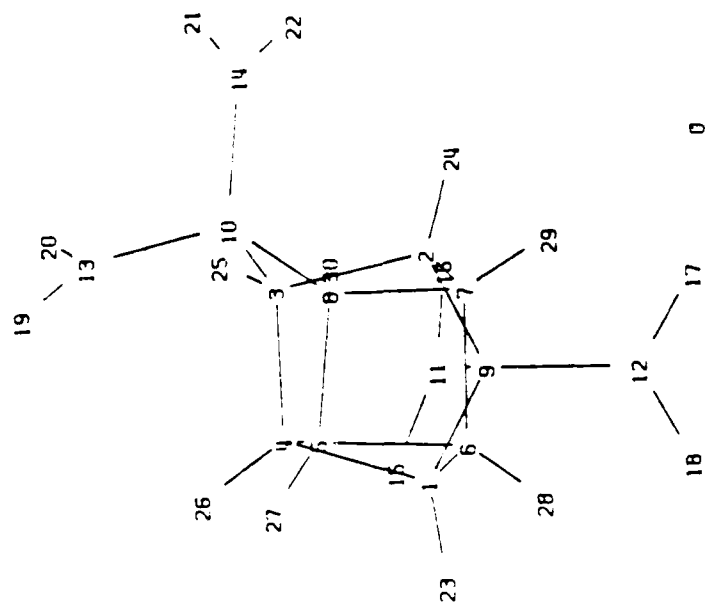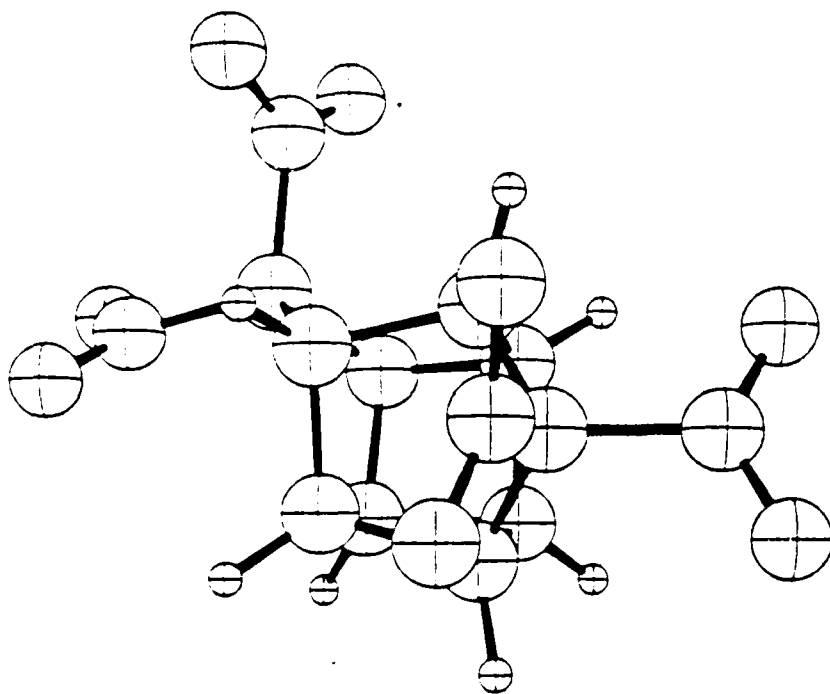
Figure A.20. 6,6,10,10-Tetranitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]-decane [Ref. A-14].

SUMMARY OF AM1 CALCULATION

VERSION 3.00

C10 H8 N4 O8   13-APR-86

Run on 6,6,10,10-tetranitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TETNPCD)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	106.990158 KCAL
ELECTRONIC ENERGY	=	-31375.469575 EV
CORE-CORE REPULSION	=	26609.912998 EV
DIPOLE	=	4.71278 DEBYE
NO. OF FILLED LEVELS	=	58
IONISATION POTENTIAL	=	12.448215 EV
MOLECULAR WEIGHT	=	312.195
SCF CALCULATIONS	=	136
COMPUTATION TIME	=	92781.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000 RESTART
Run on 6,6,10,10-tetranitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]
(TETNPCD)

C	0.000000	0	0.000000	0	0.000000	0	0	0	0
C	2.321278	1	0.000000	0	0.000000	0	1	0	0
C	1.564289	1	77.024067	1	0.000000	0	2	1	0
C	1.563136	1	100.841228	1	-12.846086	1	3		
C	1.581128	1	103.447792	1	-73.967752	1	4		
C	1.553917	1	76.293117	1	105.203547	1			
C	1.581750	1	104.017151	1	-0.376907	1			
C	1.577580	1	89.588915	1	-104.703209	1			
C	1.560841	1	101.807107	1	-46.422504	1			
C	1.561132	1	101.785517	1	-119.364399				
N	1.551320	1	112.854990	1	-64.35376				
N	1.552658	1	112.740487	1	171.91863				
N	1.552794	1	112.712866	1	171.83224				
N	1.551143	1	112.869016	1	-64.476				
O	1.192716	1	117.913488	1	129				
O	1.194144	1	117.450894						
O	1.193649	1	117.897438						
O	1.193781	1	117.63322						
O	1.193535	1	117.91264						
O	1.193796	1	117.594						
O	1.194154	1	117.46						
O	1.192805	1	117						
H	1.102346	1	114						
H	1.107706	1							
H	1.10770	1							

										CHARGE
H	1.099994	1	119.370294	1	175.551084	1	4	5	7	0.1665
H	1.093227	1	120.299032	1	-177.833591	1	5	4	2	0.1594
H	1.093200	1	120.295500	1	-177.881170	1	6	7	3	0.1594
H	1.100018	1	143.766170	1	169.082695	1	7	5	4	0.1668
H	1.102479	1	122.307798	1	-170.769419	1	8	6	1	0.1781
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C10 H8 N4 O8   13-APR-86

Run on 6,6,10,10-tetranitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TETNPCD)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	75.811337 KCAL
ELECTRONIC ENERGY	=	-30642.394198 EV
CORE-CORE REPULSION	=	26011.902094 EV
DIPOLE	=	4.60466 DEBYE
NO. OF FILLED LEVELS	=	58
IONISATION POTENTIAL	=	10.946428 EV
MOLECULAR WEIGHT	=	312.195
SCF CALCULATIONS	=	99
COMPUTATION TIME	=	78525.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000 RESTART
Run on 6,6,10,10-tetranitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane
(TETNPCD)

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.0709
C	2.281201	1	0.000000	0	0.000000	0	1	0	0	0.0645
C	1.587868	1	79.211470	1	0.000000	0	2	1	0	0.0647
C	1.586463	1	98.144065	1	-11.002045	1	3	2	1	0.0169
C	1.575981	1	102.188780	1	-77.587625	1	4	3	2	0.0063
C	1.562604	1	77.167961	1	101.756450	1	1	2	3	0.0063
C	1.575596	1	103.625434	1	-0.677199	1	6	1	2	0.0170
C	1.580813	1	90.421186	1	-105.114303	1	7	6	1	0.0707
C	1.601469	1	105.988534	1	-46.349180	1	2	3	4	-0.3244
C	1.601261	1	105.950261	1	-121.391464	1	3	2	1	-0.3244
N	1.491214	1	113.637315	1	-66.080985	1	9	2	3	1.1004
N	1.491547	1	117.179315	1	170.905115	1	9	2	3	1.1016

N	1.491498	1	117.167828	1	170.940522	1	10	3	2	1.1016
N	1.491175	1	113.653106	1	-66.012943	1	10	3	2	1.1005
.O	1.220177	1	114.852614	1	114.054667	1	11	9	2	-0.5288
O	1.222314	1	113.355800	1	-65.046057	1	11	9	2	-0.5398
O	1.219778	1	115.509633	1	11.716251	1	12	9	2	-0.5296
O	1.223062	1	112.926109	1	-167.053546	1	12	9	2	-0.5437
O	1.219781	1	115.502850	1	11.778659	1	13	10	3	-0.5296
O	1.223067	1	112.926676	1	-167.047197	1	13	10	3	-0.5437
O	1.222302	1	113.353874	1	-64.981710	1	14	10	3	-0.5398
O	1.220169	1	114.852489	1	114.099405	1	14	10	3	-0.5288
H	1.111754	1	116.372647	1	-168.616250	1	1	6	7	0.0296
H	1.113694	1	114.773475	1	159.990015	1	2	7	6	0.0225
H	1.113745	1	114.745549	1	159.952672	1	3	4	5	0.0223
H	1.108873	1	119.641494	1	177.111634	1	4	5	7	0.0348
H	1.107331	1	120.606143	1	-179.097688	1	5	4	2	0.0186
H	1.107313	1	120.612564	1	-179.167058	1	6	7	3	0.0187
H	1.108915	1	142.582971	1	170.659079	1	7	5	4	0.0347
H	1.111753	1	117.768932	1	-171.054392	1	8	6	1	0.0296
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C10 H8 N4 O8   13-APR-86

Run on 6,6,10,10-tetranitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane (TETNPCD)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	138.947782 KCAL
ELECTRONIC ENERGY	=-31018.033412 EV
CORE-CORE REPULSION	= 26238.089990 EV
DIPOLE	= 5.18351 DEBYE
NO. OF FILLED LEVELS	= 58
IONISATION POTENTIAL	= 12.523893 EV
MOLECULAR WEIGHT	= 312.195
SCF CALCULATIONS	= 67
COMPUTATION TIME	= 81824.00 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 RESTART
Run on 6,6,10,10-tetranitropentacyclo[5.3.0.0^{2,5}.0^{3,9}.0^{4,8}]decane

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(TETNPCD)

|										
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.0352
C	2.311431	1	0.000000	0	0.000000	0	1	0	0	-0.0334
C	1.588152	1	78.075109	1	0.000000	0	2	1	0	-0.0336
C	1.584699	1	99.326442	1	-11.829746	1	3	2	1	-0.0479
C	1.580112	1	102.824106	1	-75.812565	1	4	3	2	-0.0627
C	1.565190	1	76.744990	1	103.265107	1	1	2	3	-0.0622
C	1.581164	1	103.856612	1	-0.525523	1	6	1	2	-0.0483
C	1.583434	1	89.910632	1	-105.011630	1	7	6	1	-0.0351
C	1.573173	1	103.633978	1	-45.732891	1	2	3	4	0.0632
C	1.573155	1	103.632202	1	-119.722416	1	3	2	1	0.0632
N	1.559472	1	114.547020	1	-67.534451	1	9	2	3	0.4309
N	1.560804	1	115.866363	1	173.760960	1	9	2	3	0.4336
N	1.560899	1	115.861497	1	173.789746	1	10	3	2	0.4334
N	1.559385	1	114.595170	1	-67.503115	1	10	3	2	0.4308
O	1.205875	1	119.343946	1	125.926782	1	11	9	2	-0.2845
O	1.206994	1	118.326660	1	-54.620968	1	11	9	2	-0.2879
O	1.205628	1	119.576307	1	21.817439	1	12	9	2	-0.2842
O	1.207140	1	118.172628	1	-158.775469	1	12	9	2	-0.2919
O	1.205614	1	119.565081	1	22.496666	1	13	10	3	-0.2841
O	1.207121	1	118.189054	1	-158.102140	1	13	10	3	-0.2919
O	1.206972	1	118.349530	1	-54.204540	1	14	10	3	-0.2878
O	1.205888	1	119.327145	1	126.363379	1	14	10	3	-0.2845
H	1.097911	1	117.780951	1	-166.839438	1	1	6	7	0.1068
H	1.101236	1	115.418247	1	159.620343	1	2	7	6	0.1032
H	1.101290	1	115.378118	1	159.589196	1	3	4	5	0.1031
H	1.094720	1	119.707323	1	176.499109	1	4	5	7	0.0958
H	1.090309	1	120.583347	1	-178.250104	1	5	4	2	0.0941
H	1.090123	1	120.655691	1	-178.323615	1	6	7	3	0.0944
H	1.094791	1	143.184994	1	170.201453	1	7	5	4	0.0956
H	1.097849	1	119.641487	1	-170.659007	1	8	6	1	0.1070
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	
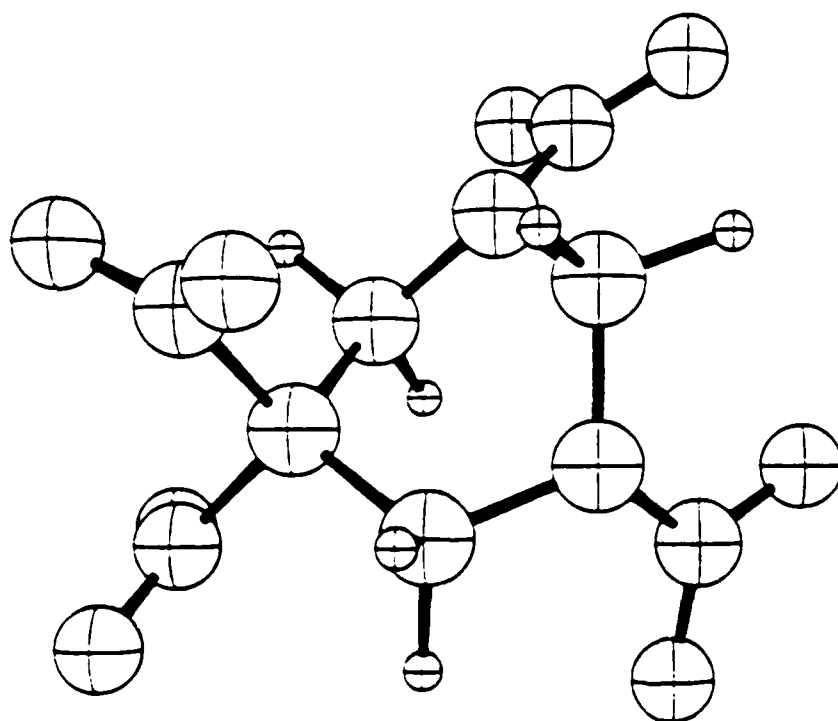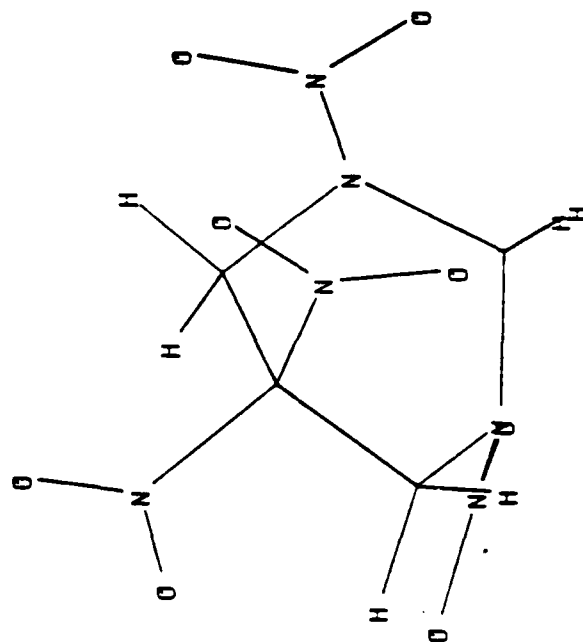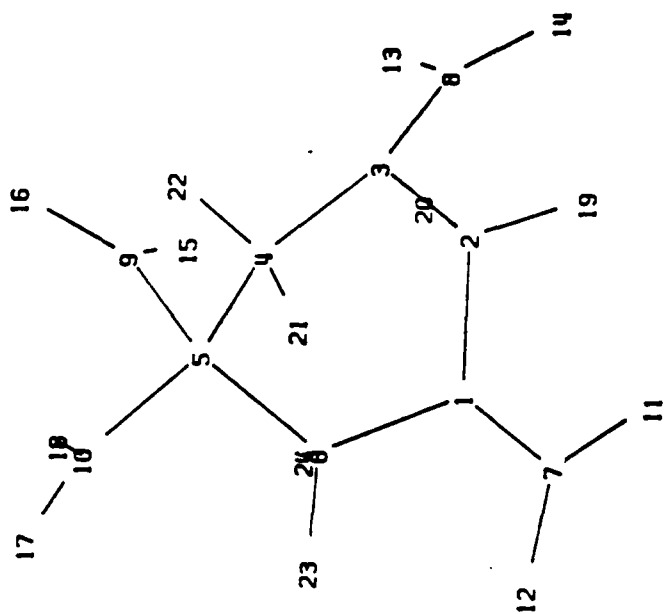
Figure A-21. 1,3,5,5-Tetranitrohexahydropyrimidine [Ref. A-15].

SUMMARY OF AM1 CALCULATION

C4 H6 N6 O8

RUN ON POTENTIAL HMX/RDX REPLACEMENT 1,3,5,5-tetranitrohexahydro-pyrimidine (DNNC)

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	88.452989 KCAL
ELECTRONIC ENERGY	=	-24913.997994 EV
CORE-CORE REPULSION	=	20529.690326 EV
DIPOLE	=	2.29587 DEBYE
NO. OF FILLED LEVELS	=	50
IONISATION POTENTIAL	=	11.985197 EV
MOLECULAR WEIGHT	=	266.127
SCF CALCULATIONS	=	855
COMPUTATION TIME	=	15897.02 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000
RUN ON POTENTIAL HMX/RDX REPLACEMENT 1,3,5,5-tetranitrohexahydro-pyrimidine (DNNC)

										CHARGE
N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.2684
C	1.470974	1	0.000000	0	0.000000	0	1	0	0	-0.0016
N	1.475946	1	115.392885	1	0.000000	0	2	1	0	-0.3174
C	1.466396	1	114.868119	1	20.841437	1	3	2	1	-0.0836
C	1.555649	1	110.791997	1	34.649899	1	4	3	2	-0.0989
C	1.563074	1	111.876163	1	-55.693268	1	5	4	3	-0.0901
N	1.427830	1	116.688719	1	81.194214	1	1	2	3	0.5949
N	1.420635	1	117.666026	1	-120.383683	1	3	2	1	0.6232
N	1.573219	1	107.626157	1	66.043891	1	5	4	3	0.5332
N	1.569581	1	109.137531	1	-176.277191	1	5	4	3	0.5358
O	1.198318	1	117.483420	1	20.843269	1	7	1	2	-0.3210
O	1.198825	1	117.947147	1	-163.197000	1	7	1	2	-0.3253
O	1.198280	1	117.581725	1	157.005807	1	8	3	2	-0.3253
O	1.196886	1	117.242989	1	-27.685812	1	8	3	2	-0.3114
O	1.193395	1	117.342493	1	-108.222652	1	9	5	4	-0.3195
O	1.190401	1	117.627374	1	69.752290	1	9	5	4	-0.2898
O	1.191709	1	116.834620	1	178.638010	1	10	5	4	-0.3001
O	1.190390	1	117.654123	1	-0.000078	1	10	5	4	-0.2930
H	1.137116	1	111.349147	1	146.715045	1	2	3	4	0.1931
H	1.137117	1	105.997822	1	-95.264457	1	2	3	4	0.1807
H	1.131001	1	112.353662	1	-86.634845	1	4	3	2	0.1429
H	1.132678	1	108.454321	1	155.310293	1	4	3	2	0.1795
H	1.131994	1	110.140819	1	-105.457793	1	6	5	4	0.1788
H	1.133518	1	110.045793	1	137.434267	1	6	5	4	0.1833

```
0     0.000000  0     0.000000  0     0.000000  0    0    0    0
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SUMMARY OF MINDO/3 CALCULATION

VERSION 3.00

C4 H6 N6 O8

RUN ON POTENTIAL HMX/RDX REPLACEMENT 1,3,5,5-tetranitrohexahydro-
pyrimidine (DNNC)

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   -24.476796 KCAL
ELECTRONIC ENERGY   =-24597.165618 EV
CORE-CORE REPULSION   = 20368.315302 EV
DIPOLE   =   5.52251 DEBYE
NO. OF FILLED LEVELS   =   50
IONISATION POTENTIAL   =   10.954194 EV
MOLECULAR WEIGHT   =   266.127
SCF CALCULATIONS   =   943
COMPUTATION TIME   = 15451.23 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY MINDO T=36000
RUN ON POTENTIAL HMX/RDX REPLACEMENT 1,3,5,5-tetranitrohexahydro-
pyrimidine (DNNC)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.3330
C	1.456264	1	0.000000	0	0.000000	0	1	0	0	0.3002
N	1.454876	1	107.053877	1	0.000000	0	2	1	0	-0.3274
C	1.461589	1	112.998366	1	-62.956233	1	3	2	1	0.2221
C	1.576075	1	112.936962	1	55.341881	1	4	3	2	-0.3525
C	1.572700	1	107.243889	1	-45.890359	1	5	4	3	0.2104
N	1.326455	1	124.703881	1	-116.506593	1	1	2	3	1.1962
N	1.331274	1	123.534386	1	120.894793	1	3	2	1	1.2016
N	1.506255	1	114.045368	1	72.454522	1	5	4	3	1.1051
N	1.514707	1	107.607928	1	-169.329084	1	5	4	3	1.1071
O	1.223645	1	114.372814	1	-11.433589	1	7	1	2	-0.5528
O	1.225124	1	114.423379	1	169.009880	1	7	1	2	-0.5657
O	1.223557	1	114.953042	1	159.524330	1	8	3	2	-0.5557
O	1.223877	1	113.820483	1	-19.048284	1	8	3	2	-0.5558
O	1.219705	1	113.872656	1	163.405879	1	9	5	4	-0.5220
O	1.220199	1	114.340162	1	-18.672536	1	9	5	4	-0.5378
O	1.220997	1	112.884388	1	-62.345536	1	10	5	4	-0.5304

O	1.217674	1	115.326488	1	115.563349	1	10	5	4	-0.5177
H	1.138702	1	109.570772	1	56.250539	1	2	3	4	-0.0434
H	1.125007	1	114.995509	1	167.181500	1	2	3	4	0.0353
H	1.131844	1	108.825028	1	-64.317687	1	4	3	2	-0.0326
H	1.122296	1	113.713427	1	-175.965628	1	4	3	2	0.0307
H	1.130150	1	109.387150	1	-69.785824	1	6	5	4	-0.0102
H	1.122399	1	113.050848	1	179.329189	1	6	5	4	0.0282
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MNDO CALCULATION

VERSION 3.00

C4 H6 N6 O8

RUN ON POTENTIAL HMX/RDX REPLACEMENT 1,3,5,5-tetranitrohexahydro-
pyrimidine (DNNC)

THE LINE MINIMISATION FAILED TWICE IN A ROW.   TAKE CARE!
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	126.972630 KCAL
ELECTRONIC ENERGY	=-24531.801713 EV
CORE-CORE REPULSION	= 20132.173404 EV
GRADIENT NORM	=	309.429789
DIPOLE	=	3.48851 DEBYE
NO. OF FILLED LEVELS	=	50
IONISATION POTENTIAL	=	12.148983 EV
MOLECULAR WEIGHT	=	266.127
SCF CALCULATIONS	=	397
COMPUTATION TIME	=	6972.70 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000
RUN ON POTENTIAL HMX/RDX REPLACEMENT 1,3,5,5-tetranitrohexahydro-
pyrimidine (DNNC)

N	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.4507
C	1.491508	1	0.000000	0	0.000000	0	1	0	0	0.3630
N	1.492144	1	112.613158	1	0.000000	0	2	1	0	-0.4592
C	1.478146	1	124.641246	1	-11.657947	1	3	2	1	0.1861
C	1.563720	1	108.867615	1	33.188281	1	4	3	2	0.0142
C	1.566276	1	108.506578	1	-58.231856	1	5	4	3	0.1799
N	1.407464	1	116.322740	1	177.639278	1	1	2	3	0.6107
N	1.406250	1	116.194057	1	-176.252303	1	3	2	1	0.6125
N	1.577224	1	112.330773	1	66.301917	1	5	4	3	0.4445

|										
N	1.576253	1	109.669547	1	-177.859389	1	5	4	3	0.4292
O	1.205018	1	117.672457	1	31.477368	1	7	1	2	-0.2908
O	1.206463	1	118.280010	1	-149.498425	1	7	1	2	-0.3081
O	1.206896	1	118.167120	1	151.512084	1	8	3	2	-0.3083
O	1.205601	1	117.790895	1	-29.567815	1	8	3	2	-0.2940
O	1.204577	1	118.733524	1	-152.040922	1	9	5	4	-0.2755
O	1.204791	1	118.727295	1	28.747386	1	9	5	4	-0.2792
O	1.203607	1	119.601683	1	-121.855759	1	10	5	4	-0.2654
O	1.207317	1	118.176055	1	58.229112	1	10	5	4	-0.2988
H	1.125083	1	109.058702	1	109.642916	1	2	3	4	0.0307
H	1.124124	1	107.816970	1	-130.533107	1	2	3	4	0.0791
H	1.121276	1	110.220603	1	-86.807981	1	4	3	2	0.0547
H	1.118261	1	110.988942	1	155.317538	1	4	3	2	0.0840
H	1.120354	1	109.599396	1	-57.618657	1	6	5	4	0.0532
H	1.117455	1	110.815743	1	-175.048791	1	6	5	4	0.0881
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

NITRAMIDE.ARC
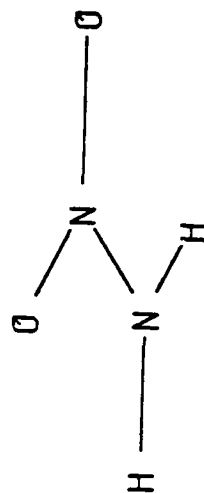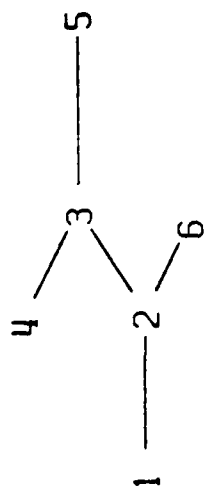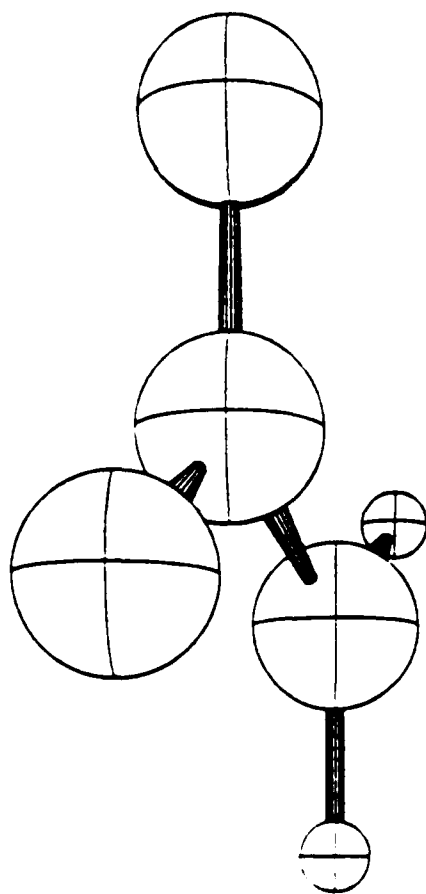
Figure A-22. Nitramide (or nitramine) [Ref. A-16]..

SUMMARY OF   AM1   CALCULATION

H2 N2 O2

17-AUG-1986 14:32:13

AM1
Run on nitramide (NH2NO2) using AM1 for comparison with other methods

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION	=	12.872749	KCAL
ELECTRONIC ENERGY	=	-2762.441360	EV
CORE-CORE REPULSION	=	1683.708120	EV
DIPOLE	=	4.19185	DEBYE
NO. OF FILLED LEVELS	=	12	
IONISATION POTENTIAL	=	12.039121	EV
MOLECULAR WEIGHT	=	62.028	
SCF CALCULATIONS	=	34	
COMPUTATION TIME	=	16.59	SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY AM1 T=36000
AM1
Run on nitramide (NH2NO2) using AM1 for comparison with other methods

Atom											Charge
H	0.000000	0	0.000000	0	0.000000	0	0	0	0		0.2688
N	0.994783	1	0.000000	0	0.000000	0	1	0	0		-0.4525
N	1.346903	1	118.120221	1	0.000000	0	2	1	0		0.6568
O	1.205562	1	117.830407	1	0.159987	1	3	2	1		-0.3710
O	1.205561	1	117.828492	1	-179.852509	1	3	2	1		-0.3710
H	0.994783	1	118.118622	1	-0.179911	1	2	3	5		0.2688
O	0.000000	0	0.000000	0	0.000000	0	0	0	0		

SUMMARY OF MINDO/3 CALCULATION

H2 N2 O2

17-AUG-1986 14:40:14

MINDO/3
Run on nitramide (NH2NO2) using MINDO for comparison with other methods

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

```
            HEAT OF FORMATION          =    -29.811557 KCAL
            ELECTRONIC ENERGY          = -2655.841021 EV
            CORE-CORE REPULSION        =  1620.894231 EV
            DIPOLE                     =     3.94629 DEBYE
            NO. OF FILLED LEVELS       =    12
            IONISATION POTENTIAL       =    11.435130 EV
            MOLECULAR WEIGHT           =    62.028
            SCF CALCULATIONS           =    34
            COMPUTATION TIME           =    10.26 SECONDS


        FINAL GEOMETRY OBTAINED                                    CHARGE
        BONDS PRECISE PULAY T=36000 MINDO
        MINDO/3
        Run on nitramide (NH2NO2) using MINDO for comparison with other methods
  H   0.000000  0    0.000000  0    0.000000  0  0  0  0      0.1385
  N   1.027358  1    0.000000  0    0.000000  0  1  0  0     -0.3262
  N   1.286985  1  125.849193  1    0.000000  0  2  1  0      1.2251
  O   1.229503  1  113.914592  1   -0.003049  1  3  2  1     -0.5880
  O   1.229502  1  113.913873  1  179.999453  1  3  2  1     -0.5880
  H   1.027357  1  125.849321  1    0.012196  1  2  3  5      0.1385
  O   0.000000  0    0.000000  0    0.000000  0  0  0  0
```

<div align="center">SUMMARY OF   MNDO   CALCULATION</div>

<div align="right">VERSION 3.10</div>

H2 N2 O2

<div align="right">17-AUG-1986 14:38:25</div>

MNDO
Run on nitramide (NH2NO2) using MNDO for comparison with other methods

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

```
            HEAT OF FORMATION          =     19.378517 KCAL
            ELECTRONIC ENERGY          = -2751.024871 EV
            CORE-CORE REPULSION        =  1667.669156 EV
            DIPOLE                     =     3.84356 DEBYE
            NO. OF FILLED LEVELS       =    12
            IONISATION POTENTIAL       =    11.943614 EV
            MOLECULAR WEIGHT           =    62.028
            SCF CALCULATIONS           =    143
            COMPUTATION TIME           =    64.02 SECONDS
```

```
         FINAL GEOMETRY OBTAINED                                 CHARGE
         BONDS PRECISE PULAY T=36000
         MNDO
         Run on nitramide (NH2NO2) using MNDO for comparison with other methods
H    0.000000  0    0.000000  0    0.000000  0   0  0  0        0.1626
N    1.017799  1    0.000000  0    0.000000  0   1  0  0       -0.2171
N    1.406534  1  112.243209  1    0.000000  0   2  1  0        0.5416
O    1.209101  1  117.850502  1  -31.072537  1   3  2  1       -0.3257
O    1.208960  1  117.773442  1  154.373111  1   3  2  1       -0.3242
H    1.017746  1  112.236434  1   33.156360  1   2  3  5        0.1627
O    0.000000  0    0.000000  0    0.000000  0   0  0  0
```

DMN.ARC
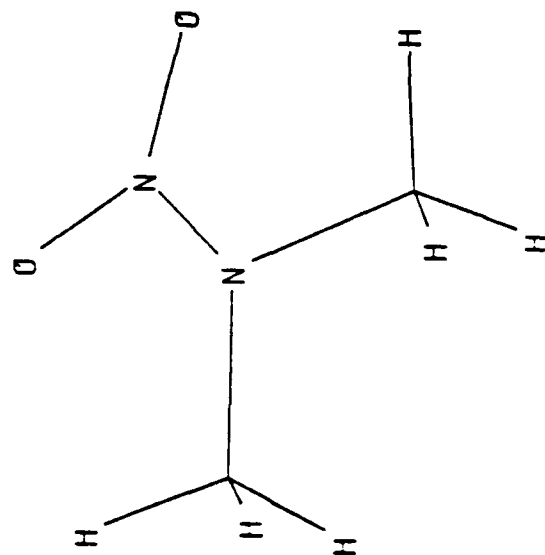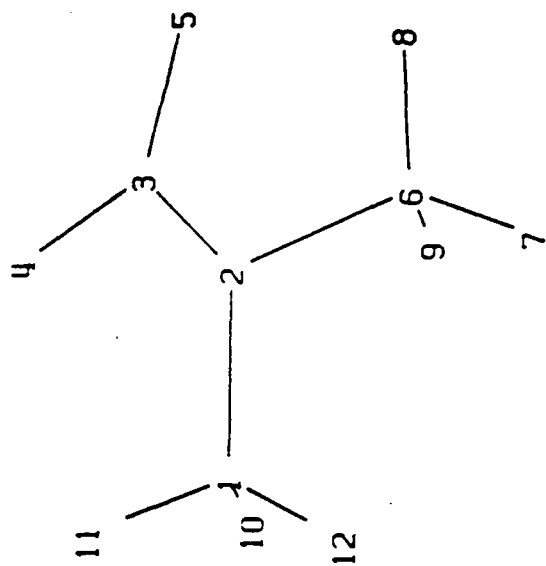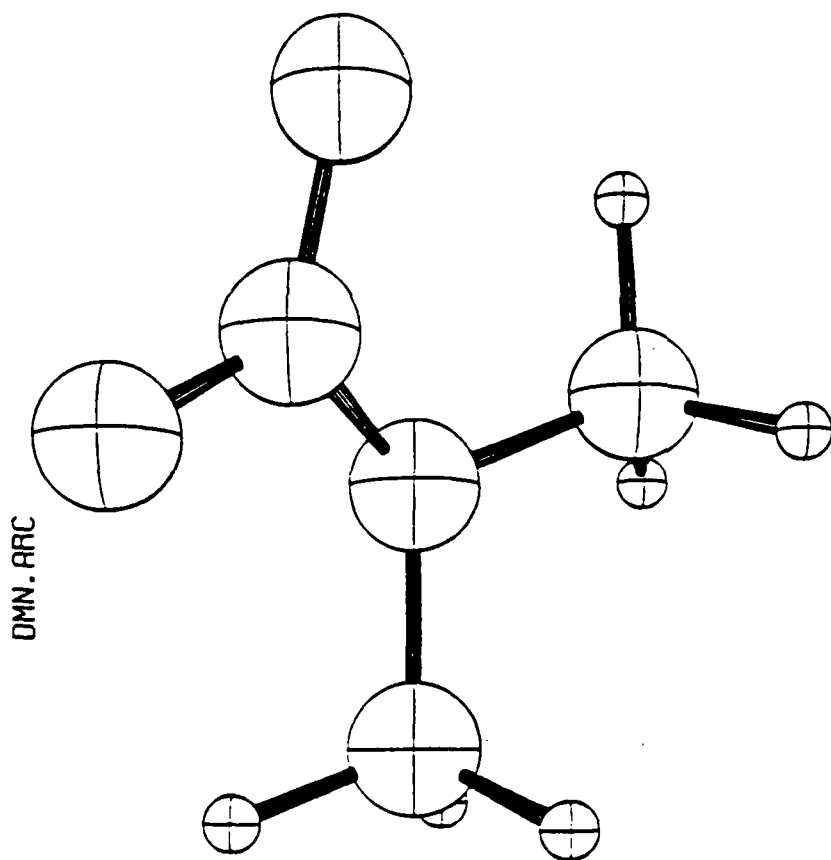
Figure A-23. Dimethylnitramide (dimethylnitramine) [Ref. A-17].

SUMMARY OF   AM1   CALCULATION

C2   H6   N2   02

12-MAR-87

AM1
Run on dimethylnitramide [N(CH3)2NO2) using AM1

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   21.704711 KCAL
ELECTRONIC ENERGY   = -4850.159974 EV
CORE-CORE REPULSION   = 3460.734479 EV
DIPOLE   =   4.62809 DEBYE
NO. OF FILLED LEVELS   =   18
IONISATION POTENTIAL   =   10.775336 EV
MOLECULAR WEIGHT   =   90.082
SCF CALCULATIONS   =   439
COMPUTATION TIME   = 3046.03 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 AM1
AM1
Run on dimethylnitramide [N(CH3)2NO2) using AM1

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	-0.1221
N	1.457823	1	0.000000	0	0.000000	0	1	0	0	-0.2724
N	1.409935	1	116.914211	1	0.000000	0	2	1	0	0.6060
O	1.202924	1	118.293439	1	-23.688765	1	3	2	1	-0.3587
O	1.202966	1	118.303052	1	161.394134	1	3	2	1	-0.3590
C	1.457771	1	116.838810	1	22.611905	1	2	3	5	-0.1217
H	1.122562	1	112.254331	1	79.770602	1	6	2	3	0.0766
H	1.122782	1	110.610879	1	-42.365109	1	6	2	3	0.1287
H	1.121774	1	106.315736	1	-160.511388	1	6	2	3	0.1085
H	1.121811	1	106.300044	1	158.791822	1	1	2	3	0.1087
H	1.122846	1	110.772673	1	40.583798	1	1	2	3	0.1294
H	1.122615	1	112.172069	1	-81.572476	1	1	2	3	0.0760
0	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF MINDO/3 CALCULATION

C2   H6   N2   02

12-MAR-87

MINDO/3

Run on dimethylnitramide [N(CH3)2NO2) using MINDO

GRADIENT TEST NOT PASSED, BUT FURTHER WORK NOT JUSTIFIED
SCF FIELD WAS ACHIEVED

HEAT OF FORMATION   =   -9.604130 KCAL
ELECTRONIC ENERGY   = -4721.312789 EV
CORE-CORE REPULSION   = 3374.424317 EV
DIPOLE   =   4.19082 DEBYE
NO. OF FILLED LEVELS   =   18
IONISATION POTENTIAL   =   10.234582 EV
MOLECULAR WEIGHT   =   90.082
SCF CALCULATIONS   =   523
COMPUTATION TIME   = 2521.35 SECONDS

FINAL GEOMETRY OBTAINED   CHARGE
BONDS PRECISE PULAY T=36000 MINDO
MINDO/3
Run on dimethylnitramide [N(CH3)2NO2) using MINDO

C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.1804
N	1.446293	1	0.000000	0	0.000000	0	1	0	0	-0.2516
N	1.310953	1	122.067814	1	0.000000	0	2	1	0	1.1743
O	1.231494	1	114.930466	1	-3.216684	1	3	2	1	-0.5927
O	1.231518	1	114.909073	1	176.843477	1	3	2	1	-0.5928
C	1.446280	1	122.090988	1	-2.563252	1	2	3	5	0.1803
H	1.118868	1	114.287949	1	69.766777	1	6	2	3	-0.0171
H	1.117758	1	114.987188	1	-53.900443	1	6	2	3	-0.0097
H	1.118258	1	111.833939	1	-171.948746	1	6	2	3	-0.0221
H	1.118700	1	114.414537	1	68.140428	1	1	2	3	-0.0159
H	1.117962	1	114.896576	1	-55.567815	1	1	2	3	-0.0111
H	1.118229	1	111.841491	1	-173.642451	1	1	2	3	-0.0220
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

SUMMARY OF   MNDO   CALCULATION

VERSION 3.10

C2 H6 N2 O2
                                                    12-MAR-87
MNDO
Run on dimethylnitramide [N(CH3)2NO2) using MNDO

HERBERTS TEST WAS SATISFIED IN FLETCHER-POWELL
SCF FIELD WAS ACHIEVED

```
HEAT OF FORMATION         =    22.878482 KCAL
ELECTRONIC ENERGY         = -4836.904615 EV
CORE-CORE REPULSION       =  3441.216413 EV
DIPOLE                    =     4.51144 DEBYE
NO. OF FILLED LEVELS      =    18
IONISATION POTENTIAL      =    11.221157 EV
MOLECULAR WEIGHT          =    90.082
SCF CALCULATIONS          =   423
COMPUTATION TIME          =  2717.79 SECONDS
```

	FINAL GEOMETRY OBTAINED									CHARGE

BONDS PRECISE PULAY T=36000
MNDO
Run on dimethylnitramide [N(CH3)2NO2) using MNDO

										CHARGE
C	0.000000	0	0.000000	0	0.000000	0	0	0	0	0.1905
N	1.486008	1	0.000000	0	0.000000	0	1	0	0	-0.3857
N	1.395073	1	117.929456	1	0.000000	0	2	1	0	0.5875
O	1.210602	1	118.608407	1	17.959739	1	3	2	1	-0.3414
O	1.210603	1	118.653406	1	-166.167914	1	3	2	1	-0.3419
C	1.485825	1	118.025170	1	-16.985083	1	2	3	5	0.1903
H	1.111804	1	111.202974	1	55.903399	1	6	2	3	0.0337
H	1.114060	1	112.431617	1	-66.894416	1	6	2	3	0.0011
H	1.112885	1	108.417061	1	173.392715	1	6	2	3	0.0156
H	1.114026	1	112.444834	1	65.121870	1	1	2	3	0.0017
H	1.111899	1	111.089645	1	-57.601504	1	1	2	3	0.0331
H	1.112783	1	108.512479	1	-175.126903	1	1	2	3	0.0155
O	0.000000	0	0.000000	0	0.000000	0	0	0	0	

APPENDIX REFERENCES

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APPENDIX B

The following file is the VAX DCL command file that submits a MOPAC job for remote execution. The file name is "MOPAC.COM".

```
$! COMMAND FILE TO SUBMIT A MOPAC JOB TO A BATCH QUEUE.
$! THIS COMMAND CAN BE USED 'MANUALLY' BY ENTERING THE INSTRUCTION
$!    "$ @MOPAC <filename> <queue> <priority>" or
$!    "$ @MOPAC" and be prompted for the other arguments,
$! A RECOMMENDED APPROACH WOULD BE TO INSERT INTO THE LOGIN COMMAND THE LINE
$!    "$ MOPAC :== @MOPACDIRECTORY:MOPAC" This would allow the command
$!
$!        "$MOPAC <filename>  <queue>  <priority>"    to be used
$!
$!    Fetch parameters
$!
$    IF P1.NES."" THEN GOTO H
$ G:
$    INQUIRE P1 "What file? "
$ H:
$    LEN = 'F$LEN(P1)'
$    DOT = 'F$LOC(".",P1)
$    IF LEN.EQ.DOT THEN GOTO CHECK
$        LEXT = LEN - DOT
$        EXT := 'F$EXT(DOT,LEXT,P1)'
$        P1 := 'F$EXT(O,DOT,P1)'
$CHECK:
$!    check to see if file is there, if not send error message
$    OPEN /ERR=NOFILE DUMMY 'P1'.DAT    ! see if data file is there
$       READ DUMMY LINE
$       YLEN = 'F$LEN(LINE)'
$       YY = 'F$LOC("RESTART",LINE)'
$    CLOSE DUMMY                                      ! Yes
$    GOTO OKAY
$NOFILE:
$    WRITE SYS$OUTPUT -
     " error opening ''P1'.DAT"
$    P1 := ""
$    GOTO G
$OKAY:
$        IF P2.EQS."" THEN P2:="RPL785_CXSLOW"
$!
$        IF P3.EQS."" THEN P3 := "2"
$!
$!    Submit
```

```
$!
$ TEMP1 := 'F$PARSE (P1+".DAT",,,"DEVICE")'
$ TEMP2 := 'F$PARSE (P1+".DAT",,,"DEVICE")''F$PARSE (P1+".DAT",,,"DIRECTORY")'
$ DIRECTT := 'F$DIRECTORY()'
$ LDIRECTT = F$LENGTH(DIRECTT)
$ LOG_FILE = DIRECTT
$ PPER = 'F$LOCATE(".",DIRECTT)'
$ IF PPER .LT. LDIRECTT THEN LOG_FILE := 'F$EXTRACT(O,PPER,DIRECTT)']
$SUBMIT /NAME='P1' USER$DISKO:[MOPAC]RMOPAC /QUEUE='P2' -
/PARA=("''P1'","''TEMP2'")/PRIO='P3'/NOTIFY -
/LOG_FILE='TEMP1''LOG_FILE''P1'.LOG/NOPRINT/RESTART
$EXIT
```

The following file is the one which actually runs the program MOPAC. It
sets up the proper logical assignments for input and output files and can be
used to run the program interactively (although this is not recommended). It is
submitted to a batch queue by the previous file, MOPAC.COM. Its name is
"RMOPAC.COM".

```
$!    COMMAND FILE TO RUN A MOPAC JOB. THIS FILE SHOULD RESIDE IN THE
$!    MOPAC DIRECTORY. IT SHOULD BE ACCESSED FROM MOPAC.COM, BUT CAN
$!    STAND ALONE, IF NECESSARY.
$!
$!    THE CALL IS          $RMOPAC filename  directory
$!
$     SHOW TIME
$!
$     SET VERIFY
$!
$!    Make assignments
$!
$     IF P2 .NES. ""       THEN SET DEFAULT 'P2'
$     ASSIGN 'P1'.END FOR004
$     ASSIGN 'P1'.DAT FOR005
$     ASSIGN 'P1'.OUT FOR006
$     ASSIGN 'P1'.RES FOR009
$     ASSIGN 'P1'.DEN FOR010
$     ASSIGN 'P1'.ARC FOR012
$     ASSIGN 'P1'.GPT FOR013
$!
$     ON ERROR   THEN GOTO AA
$     ON CONTROL_Y        THEN GOTO AA     ! Cleanup if ^Y
$     NODE = F$GETSYI("NODENAME")
$!
$!
$ WRITE SYS$OUTPUT NODE
$!
$!
$     RUN user$disk0:[MOPAC]MOPAC
$!
$     SHOW TIME
```

```
$!
$!    Delete assignments
$!
$ AA:
$     SET NOCONTROL_Y                          ! Continue cleanup if ^Y
$     DEASSIGN FORO05
$     DEASSIGN FORO06
$     DEASSIGN FORO09
$     DEASSIGN FORO10
$     DEASSIGN FORO12
$     DEASSIGN FORO13
$     SET CONTROL_Y
$     SET NOVERIFY
$!
$!    END
$!
```

The following file is used to send a MOPAC job to the FPS 164/MAX attached processor and execute it there. It is the FPS version of the RMOPAC.COM file, and is submitted by a file exactly like MOPAC.COM.

```
$!    COMMAND FILE TO RUN A MOPAC JOB. THIS FILE SHOULD RESIDE IN THE
$!    MOPAC DIRECTORY. IT SHOULD BE ACCESSED FROM MOPAC.COM, BUT CAN
$!    STAND ALONE, IF NECESSARY.
$!
$!    THE CALL IS           $RMOPAC filename  directory
$!
$     SHOW TIME
$!
$     SET VERIFY
$!
$!    Make assignments
$!
$     IF P2 .NES. ""      THEN SET DEFAULT 'P2'
$     OPEN /ERR=NOEND1 DUMMY 'P1'.END  ! see if shutdown file is there
$         DELETE/NOCONFIRM 'P1'.END;*
$NOEND1:
$     ASSIGN 'P1'.DAT FORO05
$     ASSIGN 'P1'.OUT FORO06
$     ASSIGN 'P1'.RES FORO09
$     ASSIGN 'P1'.DEN FORO10
$     ASSIGN 'P1'.ARC FORO12
$     ASSIGN 'P1'.GPT FORO13
$         ASSIGN 'P1'.END SHUTDOWN.DAT
$!
$     ON CONTROL_Y        THEN GOTO AA      ! Cleanup if ^Y
$!
$!    ATTACH TO THE FPS AND COPY IN THE FILES
$'
$ ^'E
ATTACH/W
```

```
COPYIN/B USER$DISKO:[MOPAC.FPS]MOPAC_OPT2.IMG ,MOPAC
CLEAR/ALL
MOPAC
SHOW/CPU
$
$!    SET NOVERIFY
$!
$     SHOW TIME
$!
$!    Delete assignments
$!
$ AA:
$     SET NOCONTROL_Y                         ! Continue cleanup if ^Y
$         OPEN /ERR=NOEND DUMMY 'P1'.END  ! see if shutdown file is there
$         DELETE/NOCONFIRM 'P1'.END;*
$     DEASSIGN FOR005
$     DEASSIGN FOR006
$     DEASSIGN FOR009
$     DEASSIGN FOR010
$     DEASSIGN FOR012
$     DEASSIGN FOR013
$NOEND: CLOSE DUMMY
$     SET CONTROL_Y
$     SET NOVERIFY
$!
$!    END
$!
```

The following file executes an MM2 job. It can be submitted to a batch
queue by a file exactly like MOPAC.COM. However, since MM2 generally is quite
fast, this command file is often executed by itself in interactive mode.
Several other programs are run after completion of the MM2 run. The comments in
the COM file are self-explanatory, for the most part. The CLEARBAT program
eliminates printer control characters in the first column of the output file.
The name of this file is RMM2.COM.

```
$!    COMMAND FILE TO RUN A MM2 JOB. THIS FILE SHOULD RESIDE IN THE
$!    MM2 DIRECTORY. IT SHOULD BE ACCESSED FROM MM2FAST.COM, BUT CAN
$!    STAND ALONE, IF NECESSARY.
$!
$!    THE CALL IS        $RMM2 filename  directory
$!
$     SHOW TIME
$!
$     SET VERIFY
$!
$!    Make assignments
$!
$     IF P2 .NES. ""      THEN SET DEFAULT 'P2'
$     ASSIGN 'P1'.DAT FOR008
$     ASSIGN 'P1'.LIS FOR009
```

```
$       ASSIGN 'P1'.PIC FOR013
$!
$       ON ERROR   THEN GOTO AC
$       ON CONTROL_Y      THEN GOTO AA      ! Cleanup if ^Y
$       RUN USER$DISK0:[MOLECMECH.GENERAL]MM2
$!
$!  Now run MMC and put optimized coordinates into
$!  a new .DAT file
$!
$       ASSIGN 'P1'.DAT FOR001
$       ASSIGN 'P1'.NEW FOR006
$!
$!  Now run MMC
$!
$       ON ERROR   THEN GOTO AB
$!
$       RUN USER$DISK0:[MOLECMECH.GENERAL]MMC
$!
$!  Now make the new data file the most current version
$!  and delete the old version
$!
$       RENAME 'P1'.NEW 'P1'.DAT
$       GOTO AC
$!
$ AB:
$!
$       RENAME FOR007.DAT 'P1'.COR
$!
$ AC:
$!
$!       Clean up the output file for proper display
$!
$       ON ERROR   THEN GOTO AA
$!
$       ASSIGN 'P1'.LIS FOR001
$       ASSIGN 'P1'.NEW FOR006
$       RUN USER$DISK0:[MOLECMECH.GENERAL]CLEARBAT
$       RENAME 'P1'.NEW 'P1'.LIS
$!
$!
$       SHOW TIME
$!
$!  Delete assignments
$!
$ AA:
$       SET NOCONTROL_Y                        ! Continue cleanup if ^Y
$       DEL FOR012.DAT;1
$       DEL FOR007.DAT;1
$       DEASSIGN FOR001
$       DEASSIGN FOR006
$       DEASSIGN FOR008
$       DEASSIGN FOR009
$       DEASSIGN FOR013
$       SET CONTROL_Y
```

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```
$    SET NOVERIFY
$!
$!   END
$!




     The following command file is designed to execute a GAMESS job.  It is
submitted to a batch queue by a file exactly like MOPAC.COM.  Its name is
RGAMESS.COM.


$!   COMMAND FILE TO RUN A GAMESS JOB. THIS FILE SHOULD RESIDE IN THE
$!   GAMESS DIRECTORY. IT SHOULD BE ACCESSED FROM GAMESS.COM, BUT CAN
$!   STAND ALONE, IF NECESSARY.
$!
$!   THE CALL IS          $RGAMESS filename  directory
$!
$    SHOW TIME
$!
$    SET VERIFY
$ ON ERROR THEN GOTO AA
$ ON CONTROL_Y THEN GOTO AA
$!
$!   Make assignments
$!
$    IF P2 .NES. ""      THEN SET DEFAULT 'P2'
$ assign user$disk11:[scratch] scr
$ NAME = F$EXT(0,15,P1)
$ SET PROCESS/NAME='NAME'
$ COPY 'P1'.INP SCR:'P1'.F05    ! Pick up the input data
$ ASSIGN SCR:'P1'.IRC   IRCDATA
$ ASSIGN SCR:'P1'.F05   INPUT
$ ASSIGN SYS$OUTPUT     OUTPUT
$ ASSIGN SCR:'P1'.DAT   PUNCH
$ ASSIGN SCR:'P1'.F08   INTGRLS
$ ASSIGN SCR:'P1'.F09   ORDINT
$ ASSIGN SCR:'P1'.F09   JKFILE
$ ASSIGN SCR:'P1'.F10   DICTNRY
$ ASSIGN SCR:'P1'.F11   DRTFILE
$ ASSIGN SCR:'P1'.F12   CIVECTR
$ ASSIGN SCR:'P1'.F15   WORK15
$ ASSIGN SCR:'P1'.F16   WORK16
$ ASSIGN SCR:'P1'.F20   DASORT
$!
$!
$!
$ NODE = F$GETSYI("NODENAME")
$!
$!
$ WRITE SYS$OUTPUT NODE
$!
$!
$ RUN user$disk1:[g82.gamess]GAMESS
```

```
$ DIRECTORY/SIZE=ALL/DATE SCR:'P1'.*
$ COPY SCR:'P1'.DAT 'P2''P1'.ARC
$ DEL SCR:'P1'.DAT;*
$!
$    SHOW TIME
$!
$!   Delete assignments
$!
$ AA:
$    SET NOCONTROL_Y                          ! Continue cleanup if ^Y
$ DEASSIGN IRCDATA
$ DEASSIGN INPUT
$ DEASSIGN OUTPUT
$ DEASSIGN PUNCH
$ DEASSIGN INTGRLS
$ DEASSIGN ORDINT
$ DEASSIGN JKFILE
$ DEASSIGN DICTNRY
$ DEASSIGN DRTFILE
$ DEASSIGN CIVECTR
$ DEASSIGN WORK15
$ DEASSIGN WORK16
$ DEASSIGN DASORT
$    SET CONTROL_Y
$    SET NOVERIFY
$!              '
$!   END
$!
```

The following file runs a GAMESS job on the FPS-164/MAX attached processor. It is submitted to a batch queue by a file just like MOPAC.COM. Its name is RGAMESS_FPS.COM.

```
$!   COMMAND FILE TO RUN AN FPS GAMESS JOB. THIS FILE SHOULD RESIDE IN THE
$!   GAMESS DIRECTORY. IT SHOULD BE ACCESSED FROM GAMESS.COM, BUT CAN
$!   STAND ALONE, IF NECESSARY.
$!
$!   THE CALL IS          $RGAMESS_FPS filename  directory
$!
$    SHOW TIME
$!
$    SET VERIFY
$ ON ERROR THEN GOTO AA
$ ON CONTROL_Y THEN GOTO AA
$!
$!   Make assignments
$!
$    IF P2 .NES. ""      THEN SET DEFAULT 'P2'
$ assign user$disk11:[scratch.fps_scratch] scr
$ NAME = F$EXT(0,15,P1)
$ SET PROCESS/NAME='NAME'
```

```
$ COPY 'P1'.INP SCR:'P1'.F05      ! Pick up the input data
$ ASSIGN SCR:'P1'.IRC   IRCDATA
$ ASSIGN SCR:'P1'.F05   INPUT
$ ASSIGN SYS$OUTPUT     OUTPUT
$ ASSIGN SCR:'P1'.DAT   PUNCH
$ ASSIGN SCR:'P1'.F08   INTGRLS
$ ASSIGN SCR:'P1'.F09   ORDINT
$ ASSIGN SCR:'P1'.F09   JKFILE
$ ASSIGN SCR:'P1'.F10   DICTNRY
$ ASSIGN SCR:'P1'.F11   DRTFILE
$ ASSIGN SCR:'P1'.F12   CIVECTR
$ ASSIGN SCR:'P1'.F15   WORK15
$ ASSIGN SCR:'P1'.F16   WORK16
$ ASSIGN SCR:'P1'.F20   DASORT
$!
$! Go to the FPS
$!
$ SJE/TIME/CONTINUE
      ATTACH/WAIT/TMRAM
      COPYIN INPUT,INPUT
      COPYIN/B USER$DISK1:[G82.GAMESS]GAMES.IMG,GAMESS
      DIR
      CLEAR/ALL
      SHOW/CPU
      GAMESS
      SHOW/CPU
      COPYOUT PUNCH,PUNCH
      COPYOUT/B IRCDATA,IRCDATA
      COPYOUT/B INTGRLS,INTGRLS
      COPYOUT/B ORDINT,ORDINT
      COPYOUT/B JKFILE,JKFILE
      COPYOUT/B DICTNRY,DICTNRY
      COPYOUT/B DRTFILE,DRTFILE
      COPYOUT/B CIVECTR,CIVECTR
      COPYOUT/B WORK15,WORK15
      COPYOUT/B WORK16,WORK16
      COPYOUT/B DASORT,DASORT
      DETACH;QUIT
$ DIRECTORY/SIZE=ALL/DATE SCR:'P1'.*
$ COPY SCR:'P1'.DAT 'P2''P1'.ARC
$ DEL SCR:'P1'.DAT;*
$!
$     SHOW TIME
$!
$!    Delete assignments
$!
$ AA:
$     SET NOCONTROL_Y                      ! Continue cleanup if ^Y
$ DEASSIGN IRCDATA
$ DEASSIGN INPUT
$ DEASSIGN OUTPUT
$ DEASSIGN PUNCH
$ DEASSIGN INTGRLS
$ DEASSIGN ORDINT
```

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```
$ DEASSIGN JKFILE
$ DEASSIGN DICTNRY
$ DEASSIGN DRTFILE
$ DEASSIGN CIVECTR
$ DEASSIGN WORK15
$ DEASSIGN WORK16
$ DEASSIGN DASORT
$    SET CONTROL_Y
$    SET NOVERIFY
$!
$!   END
$!
```

END

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